IDAES Integrated Platform for Multi-Scale Modeling and Optimization

Tony Burgard & Debangsu Bhattacharyya

April 23, 2024

IDAES Overview

- IDAES is an open-source, equation-oriented software platform, written in Pyomo (Python-based), that enables the design and optimization of multi-scale, dynamic, interacting technologies and systems.
- Objective: Accelerate design & deployment of integrated power, H_2, and industrial processes to support broad decarbonization and emerging R&D priorities.

Also see: Overview – IDAES

More in-depth overview: Energy Institute Lecture Series: Dr. David C. Miller – Texas A&M Energy Institute (tamu.edu)

On-line documentation:
Institute for the Design of Advanced Energy Systems (IDAES) — IDAES v2.4.0 (idaes-pse.readthedocs.io)

- Major Focus Areas:
  1. Growing the user base in strategic areas
  2. Ensuring that existing projects leveraging IDAES are successful
  3. Continuing to build out advanced capabilities

Several Modeling Collaborations Now Use IDAES

Project	Application	Sponsor	Partners
IDAES – Institute for the Design of Advanced Energy Systems	H_2 with Capture	*FECM*	National Energy Technology Laboratory; Berkeley Lab; Sandia National Laboratories; Carnegie Mellon; West Virginia University; University of Notre Dame; Georgia Tech
CCSI² – Carbon Capture Simulation for Industry Impact	Post-Combustion Carbon Capture/CDR	*FECM*	National Energy Technology Laboratory; Berkeley Lab; Lawrence Livermore National Laboratory; Los Alamos National Laboratory; Pacific Northwest National Laboratory; Oak Ridge National Laboratory; West Virginia University; University of Notre Dame; The University of Texas at Austin; UT; University of Pittsburgh; Carnegie Mellon
DISPATCHES – Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems	Hybrid Energy Systems	*FECM, NE, EERE via GMLC*	National Energy Technology Laboratory; Sandia National Laboratories; Berkeley Lab; INL Idaho National Laboratory; NREL Transforming ENERGY; University of Notre Dame
PROMMIS – Process Optimization and Modeling for Minerals Sustainability	Rare Earth Element & Critical Mineral Recovery	*BIL via FECM*	National Energy Technology Laboratory; Berkeley Lab; Sandia National Laboratories; Carnegie Mellon; West Virginia University; University of Notre Dame; Georgia Tech
WaterTAP	Water Desalination	*EERE via NAWI & IEDO*	National Energy Technology Laboratory; Berkeley Lab; NREL Transforming ENERGY; Oak Ridge National Laboratory
PARETO – The Produced Water Optimization Initiative	Produced Water Management	*FECM*	National Energy Technology Laboratory; Berkeley Lab; Carnegie Mellon; Georgia Tech

IDAES Integrated Platform

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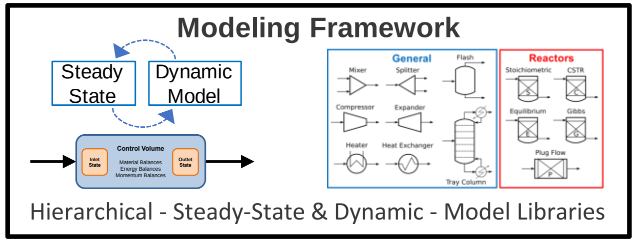
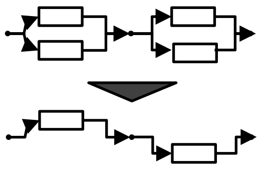
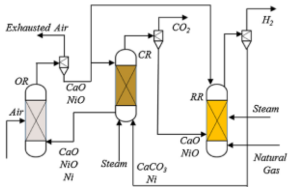


Conceptual Design

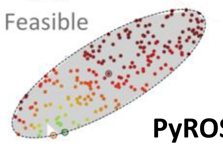


PYOMO GDP

Plant Design Process Optimization



Uncertainty Quantification Robust Optimization

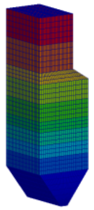


PyROS

AI/ML Surrogate Modeling

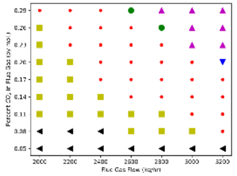
ALAMO a black-box modeling tool

PySMO

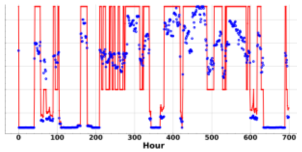


Infrastructure Planning of Reliable Carbon Neutral Power Systems

Process Family Design

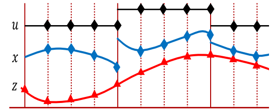


Process/Market Co-Optimization



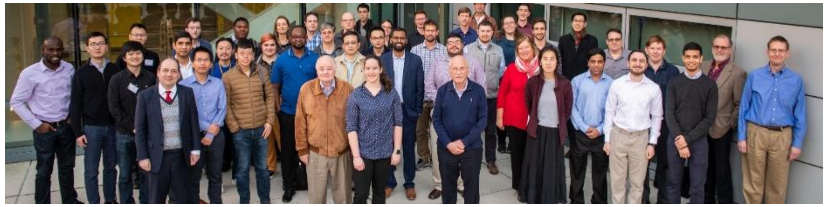
Process Operations Dynamics & Control

caprese



Open Source: https://github.com/IDAES/idaes-pse

Lee, et al., *J. of Adv. Manufacturing and Processing* (2021)



2020 R&D 100 WINNER

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Sandia National Laboratories

Carnegie Mellon

West Virginia University

UNIVERSITY OF NOTRE DAME

Georgia Tech

PYOMO

python™

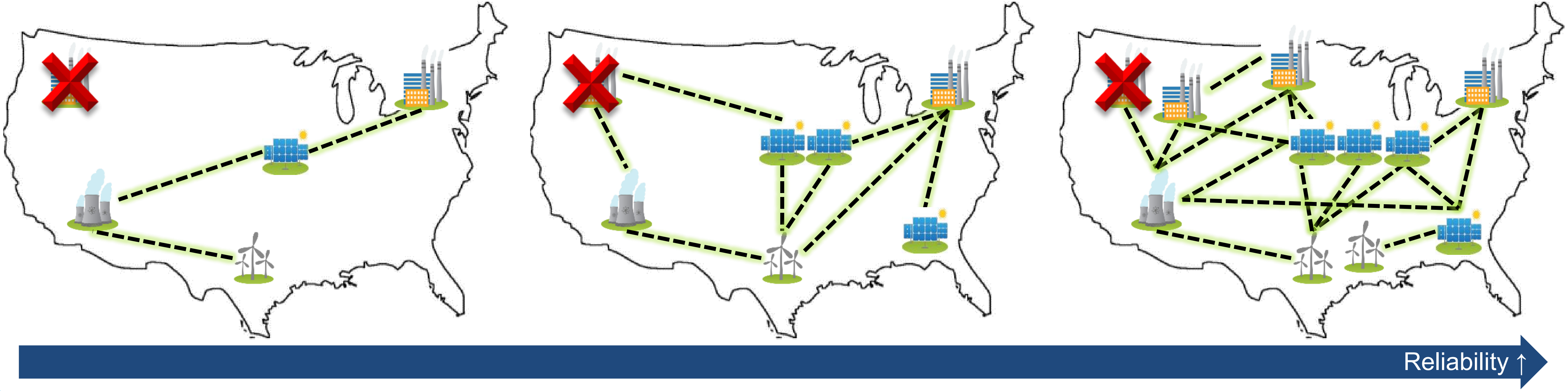
Gurobi	CPLEX	Xpress	CBC	Ipopt
GAMS	NEOS	Mosek	BARON	GLPK

IDAES New Capability Development

- **Infrastructure planning of reliable and carbon-neutral power systems**
- Integrating manufacturing considerations into process design
- Integrated process market optimization of power and H_2 systems
- Dynamics, control, health modeling and optimization of power and H_2 systems

Infrastructure Planning of Reliable & Carbon-Neutral Power Systems

- **Objective**
  - To determine long-term (yearly) investment decisions (time, location, number of power facilities) while considering short-term (hourly) operation decisions and explicitly valuing power system reliability.
- **Research challenge**
  - How to solve these problems at a meaningful scale!
  - Simplifications (e.g., representative days, ignoring reliability penalties, storage, and uncertainty) and scale reductions (e.g., short time horizons, small regions, clustering of generators) are needed to make the problems solvable but limit their usefulness for long-term decision making.



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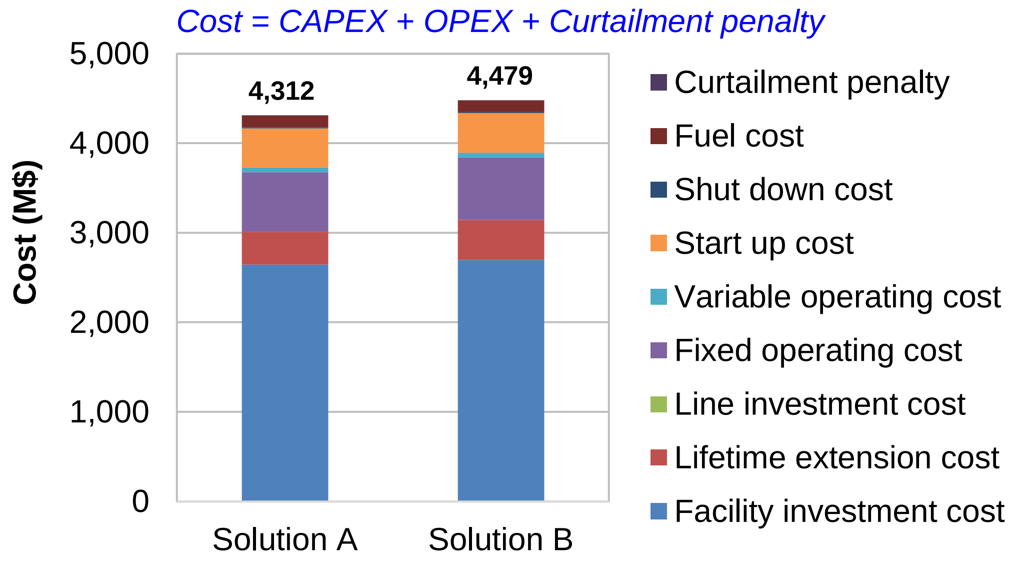
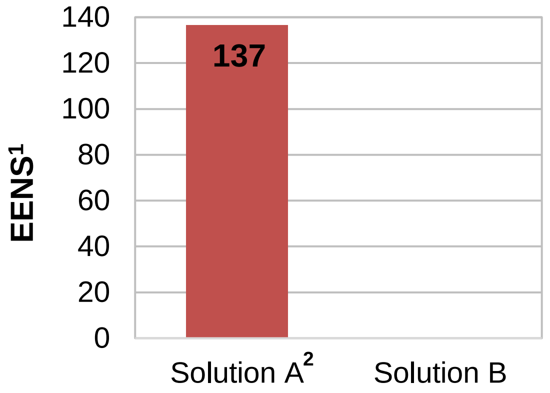
Cho, et al., *Computers & Chemical Engineering*, 2023

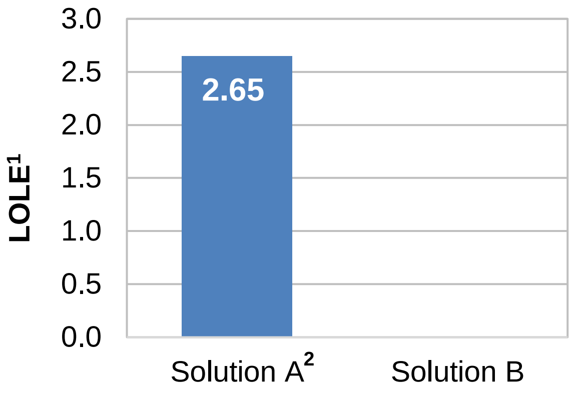
San Diego County Case Study: Why consider reliability?

California Policy and Regulatory Environment	Scenario #1	Scenario #2	Scenario #3
CO_2 emission limits (30% reduction by Y10)	X	O	O
Renewable generation (60% of the total generation by Y10)	X	X	O

Solution A: Results of expansion planning **without** reliability consideration
Solution B: Results of expansion planning **with** reliability consideration





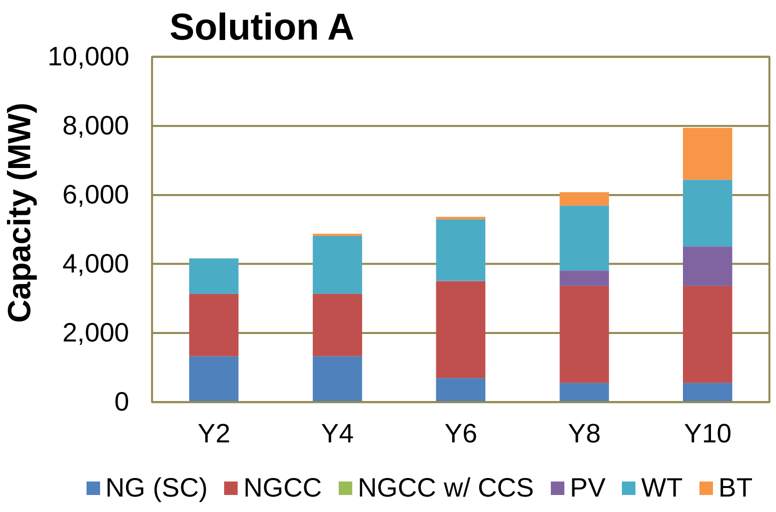


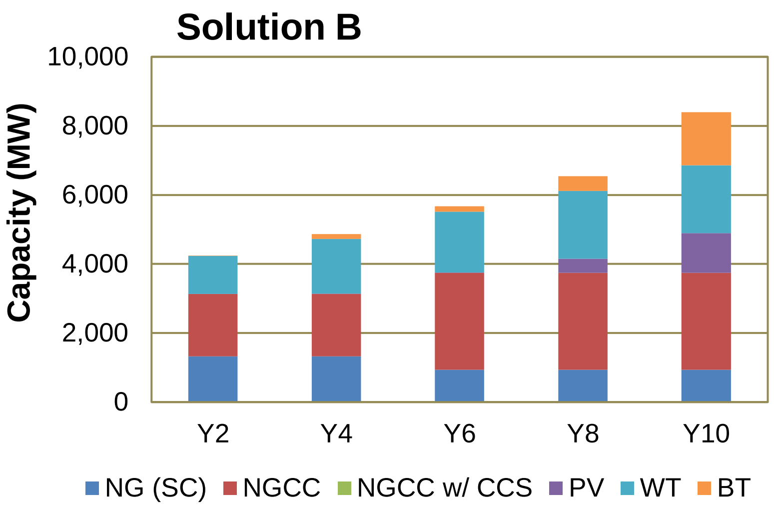
[1] EENS (MWh/planning period) and LOLE (hours/planning period) over 10 years are estimated.
[2] LOLE and EENS of solution A are analyzed after obtaining the optimal configuration.
Higher EENS and LOLE indicate the power system has a relatively lower reliability level.

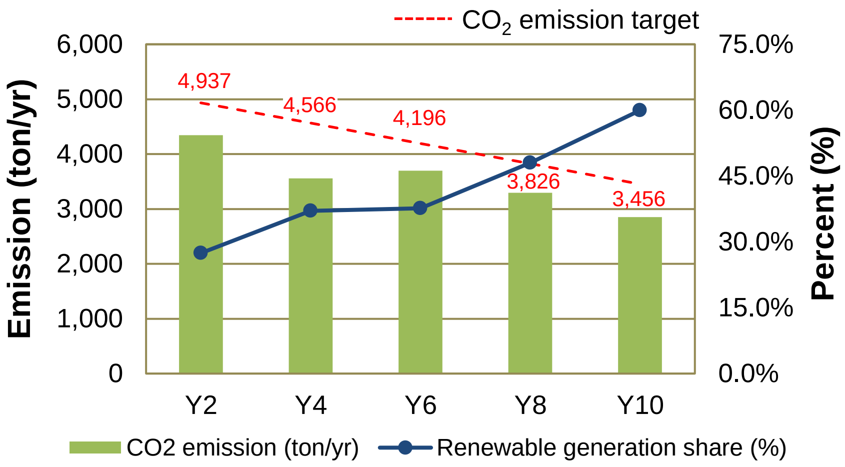
The framework enables users to estimate cost of designing power systems that can flexibly respond to failures.

San Diego County Case Study: What leads to reliability improvement?

Solution A: Results of expansion planning **without** reliability consideration
Solution B: Results of expansion planning **with** reliability consideration







- Primary means of improving reliability was extending lifetimes of NG simple cycle plants to serve as back-ups.

- Capacity of renewable generators, which have lower failure rates than dispatchable generators, is also increased, albeit minimally.

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IDAES New Capability Development

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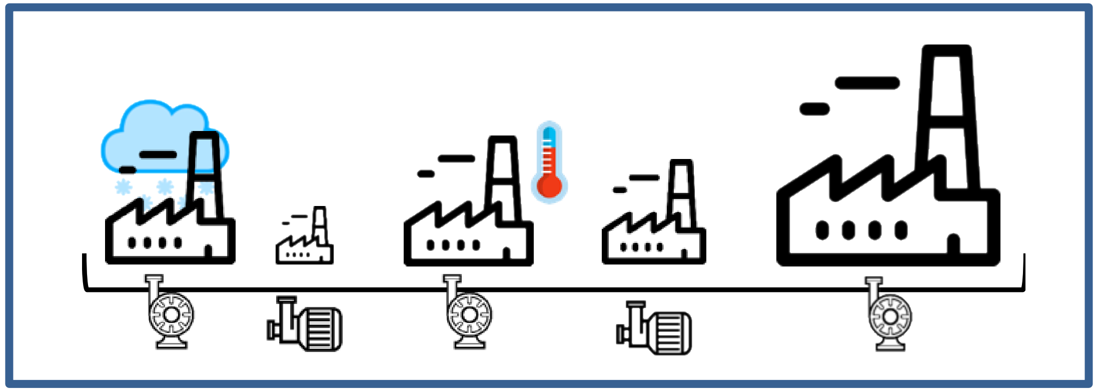
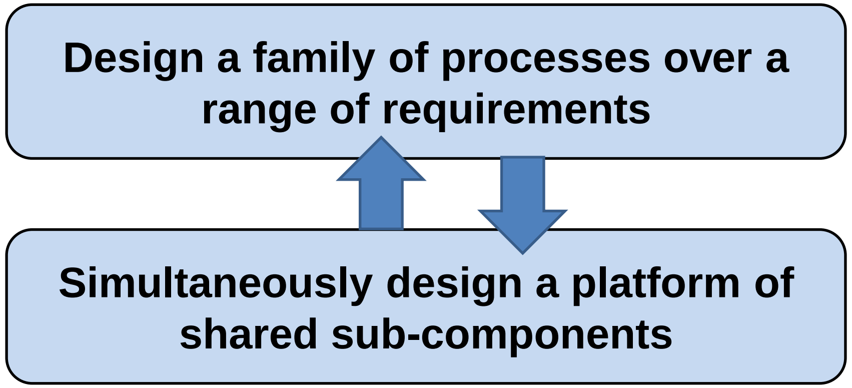
Optimization Approaches for Rapid Design and Deployment of Industrial Decarbonization Processes

- **Objective**
  - Simultaneously design families of processes able to address a wide range of operating conditions and performance requirements, that maximize the use of shared sub-components/unit operations.
- **Why does this matter?**
  - De-risks large-scale deployments by explicitly integrating manufacturing considerations into design
  - Reduces both deployment times (since fewer units will require custom design & fabrication) and manufacturing costs (by exploiting economies of learning since we produce a larger number of each of the units)



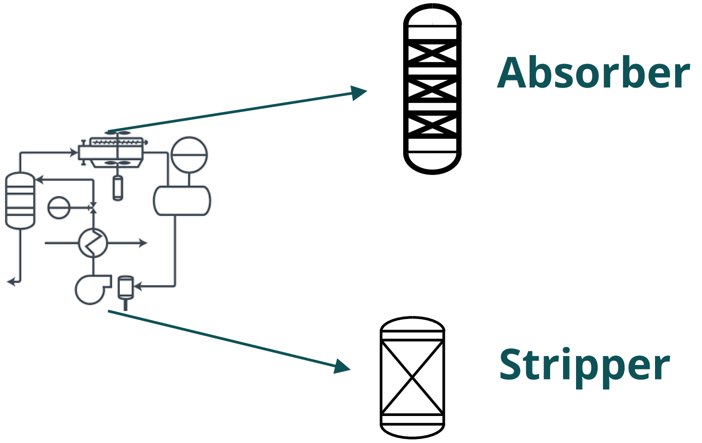


Stinchfield, et. al., *Computers Aided Chemical Engineering*, 2023
Stinchfield, et. al., *Computers & Chemical Engineering*, 2024

Case Study: MEA Carbon Capture

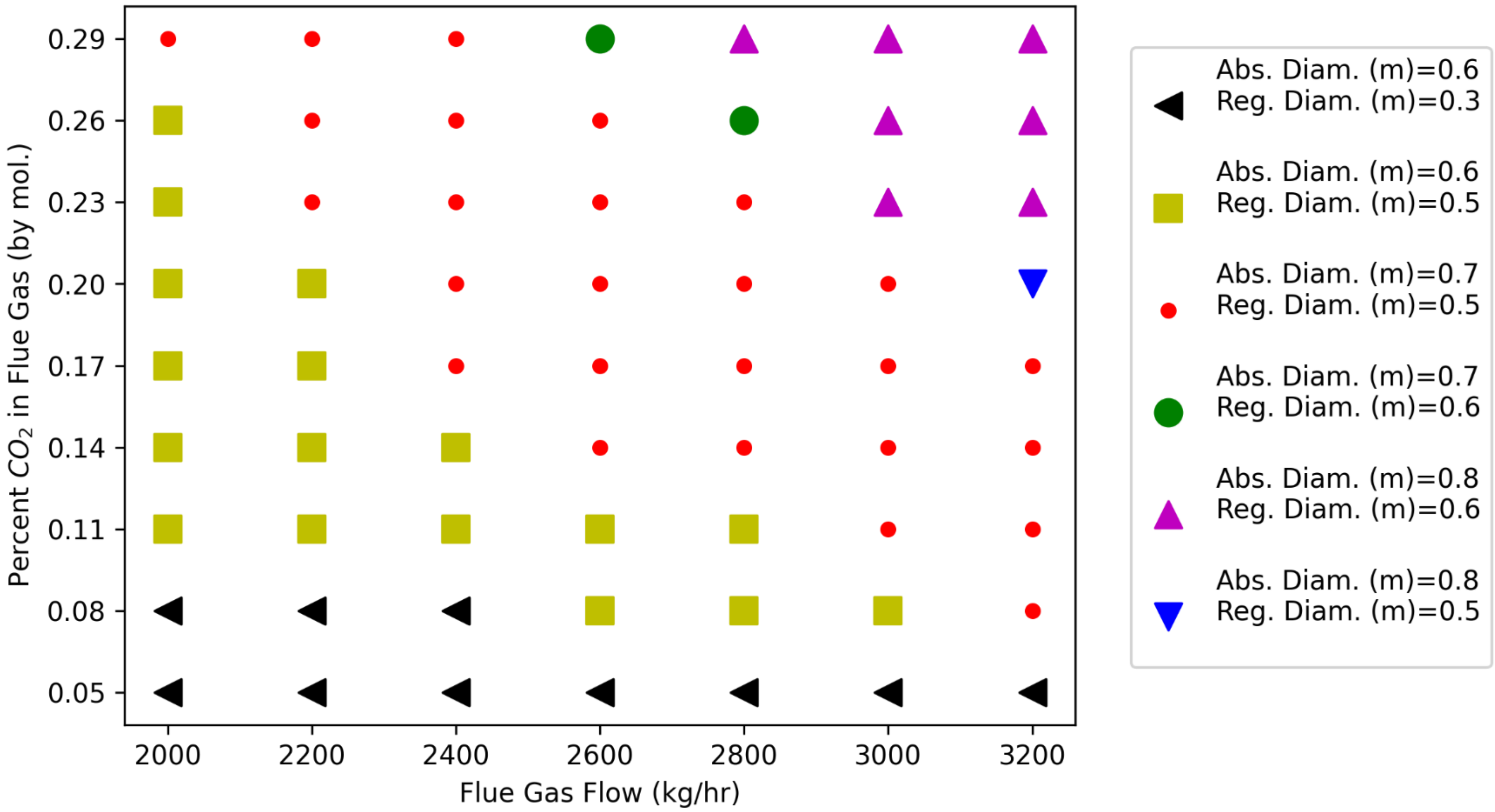
Successfully designed 63 carbon capture systems using only 3 optimally designed absorbers & strippers

Units designed to be **shared**



Absorber Ranges
0.3 – 1.2 (by 0.1's) m. diameter

Stripper Ranges
10 – 55 (by 5's) in. diameter



Total cost savings (economies of numbers) estimated to be **14.3%**

- Currently using literature values for economies of numbers savings
- Investigating specific parameters for CO2 capture processes

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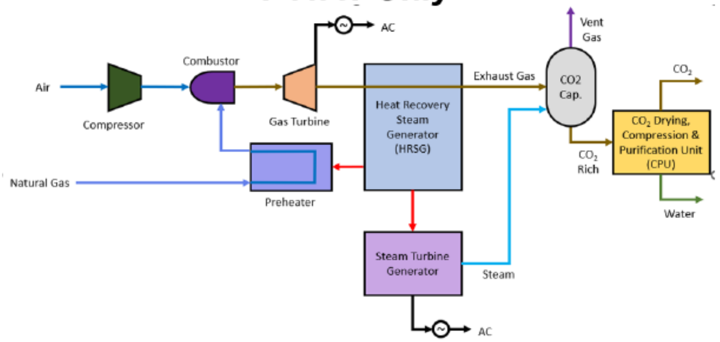
Analysis of Integrated Energy System Concepts

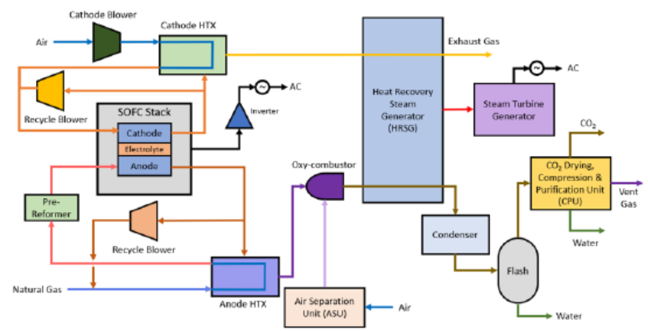
Fuel = Natural Gas
CO_2 capture > 97%

Baseline Systems
Single Product

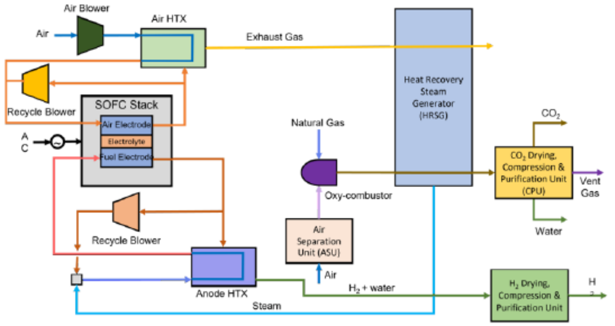
Standalone Natural Gas Combined Cycle (NGCC)
Power Only



Standalone Solid Oxide Fuel Cell (SOFC)
Power Only

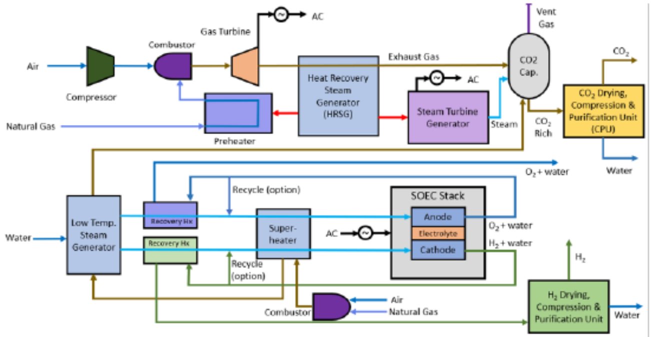


Standalone Solid Oxide Electrolyzer Cell (SOEC)
Hydrogen Only

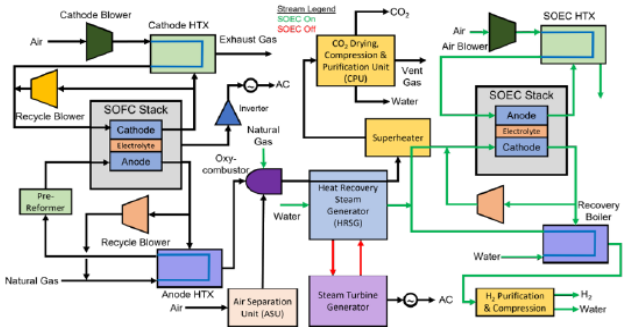


Integrated Systems
Multi-Product

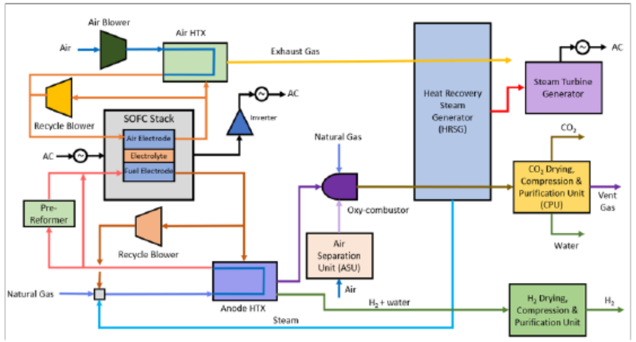
NGCC + SOEC
Power, Hydrogen, Coproduction



SOFC + SOEC
Power, Hydrogen, Coproduction



Reversible Solid Oxide Cell (rSOC)
Power, Hydrogen



Are there plausible electricity market scenarios where an integrated system makes sense?
If so, which system is the best?

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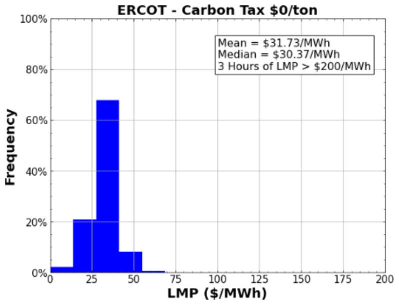
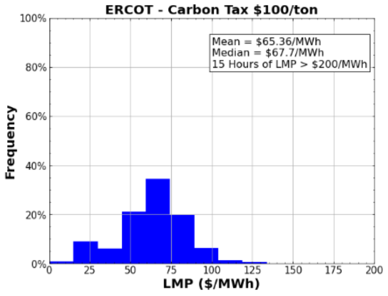
Analysis of Flexible Power and H_2 Systems

- **Systems Under Evaluation** All > 97% CO2 Capture
  - Single Product: NGCC, SOFC, SOEC
  - Multi Product: NGCC+SOEC, SOFC+SOEC, rSOC
- **61 total data sets** (every hour for a year)
  - 2019 & 2022: ERCOT, ISO_NE, MISO, PJM, SPP, NYISO
  - Future projections from NREL and Princeton from ARPA-E FLECCS program
  - Future projections from NETL for ERCOT using PROMOD IV

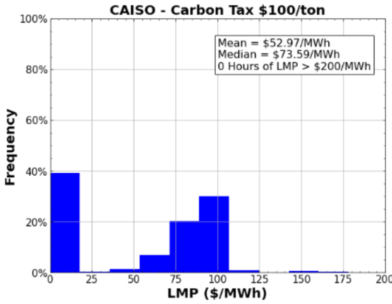
Data sets cover very broad range of potential scenarios



Low Prices



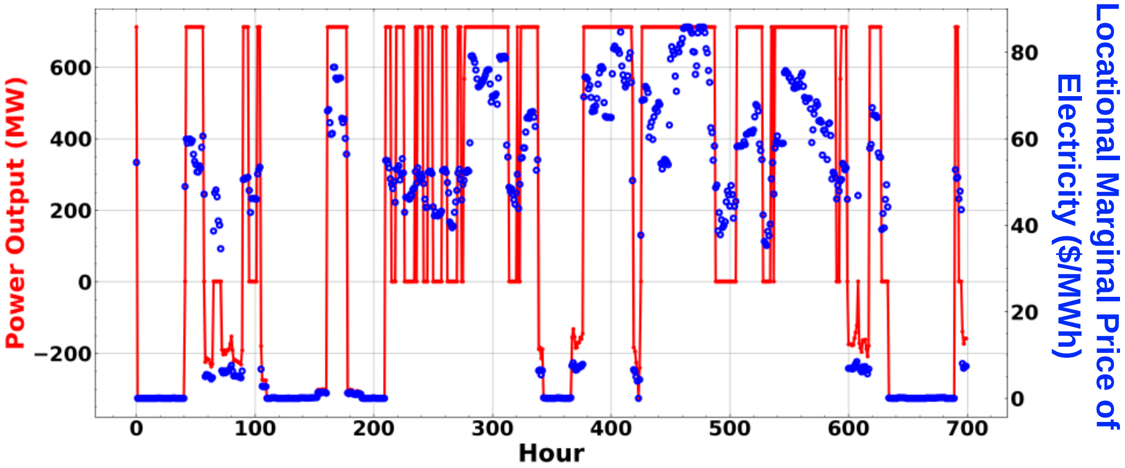
High Prices

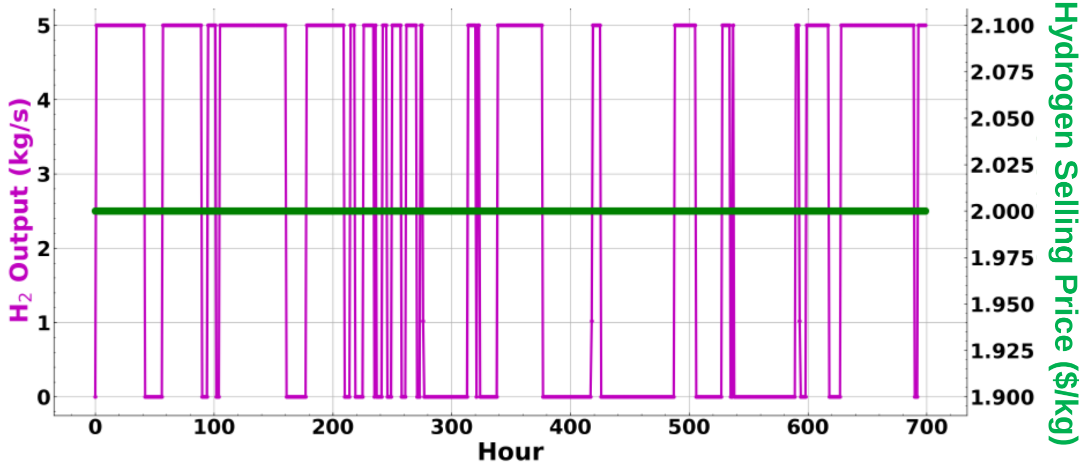


Bimodal (e.g., high VRE)

Optimize IES Operation

$$\max \sum (\text{Revenue}_t - \text{Costs}_t - CO_2\text{Tax}_t)$$





Eslick, et. al., DOE/NETL-2023/4322

Laky, et. al., 2024, *to be submitted*

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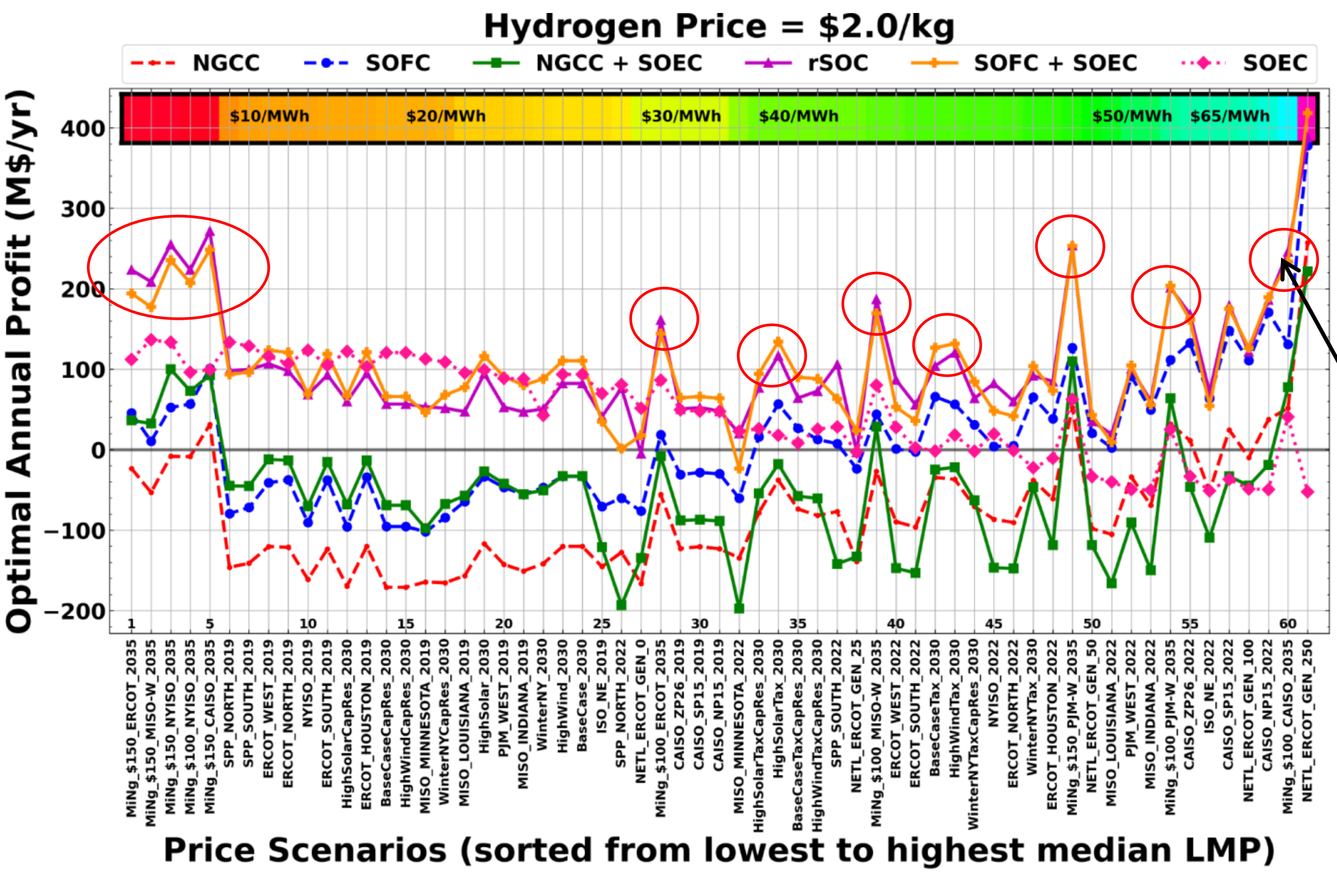
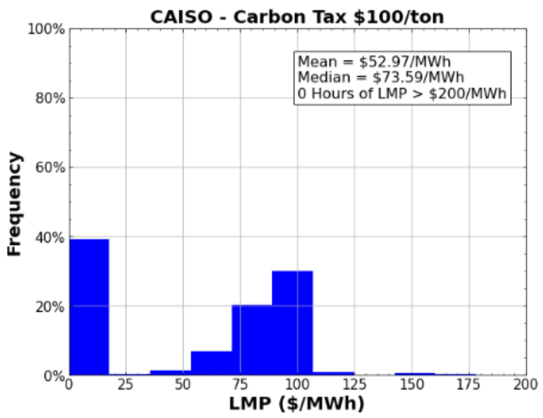
Flexible Power/H_2 Systems Outperform Single Product Systems



% of electricity market **scenarios with positive annualized profit** assuming $2/kg H_2 selling price

NGCC (power only)	13%
SOFC (power only)	52%
SOEC (H2 only)	74%
NGCC + SOEC (power and/or H2)	16%
Reversible SOC (power or H2)	97%
SOFC + SOEC (power and/or H2)	98%

Integrated power and hydrogen systems are the most robust to electricity market assumptions.



How might we control these systems to switch between operating modes while minimizing degradation over long-term operation?

Integrated power and hydrogen systems provide greatest benefits in scenarios with bimodal electricity pricing (e.g., high VRE).

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- Infrastructure planning of reliable and carbon-neutral power systems
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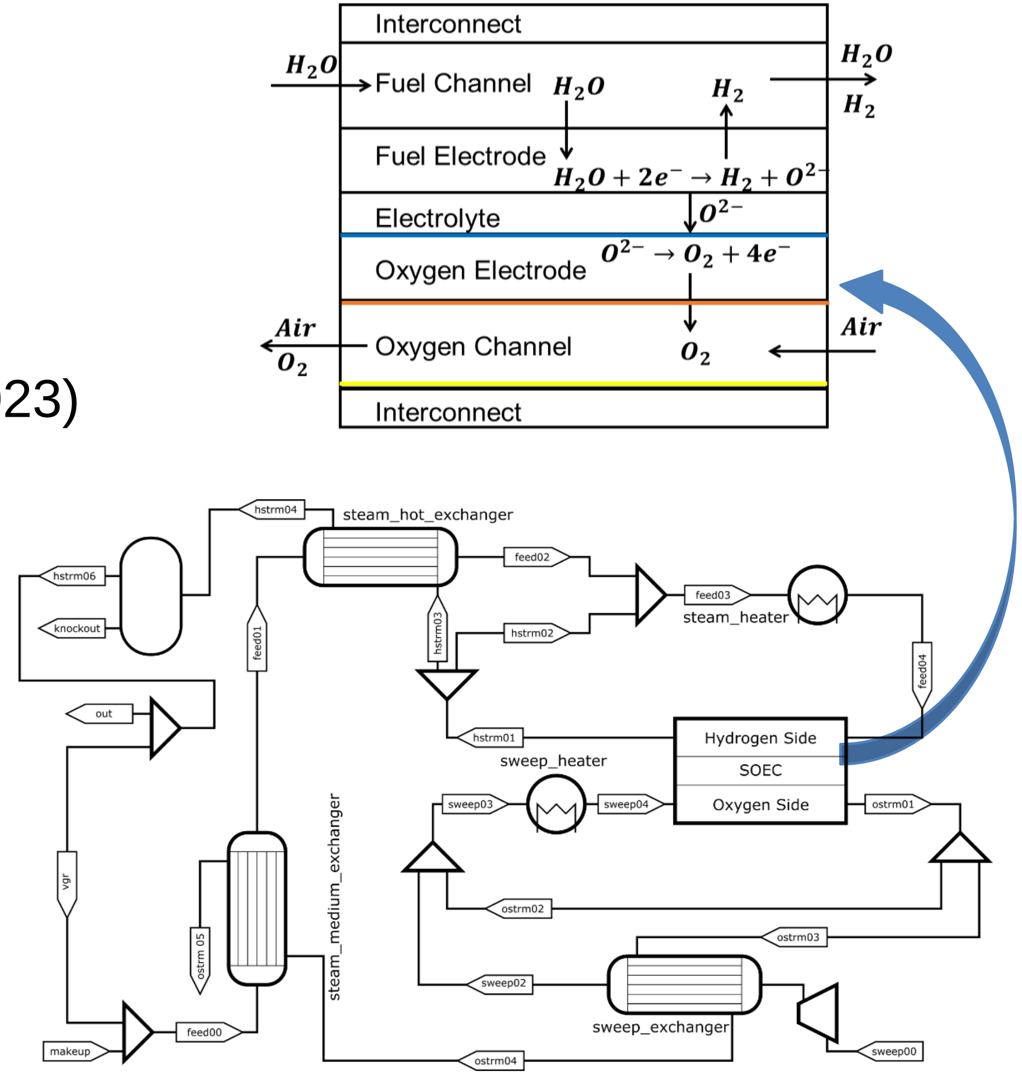
- **Dynamics, control, health modeling & optimization of power and H_2 systems**

Dynamic Model of SOC-based System for Mode-Switching

- **SOC dynamic model** (Bhattacharyya et al., 2007)
  - First-principles, non-isothermal, planar cell
  - 2D electrodes, electrolyte, and interconnect
  - 1D fuel and oxygen channels
  - Operates in fuel cell and electrolysis modes
- **Dynamic SOC-based system model** (Allan et al., 2023)
  - Now [publicly available online]
    - Soon to be merged into the IDAES examples repository
  - **H_2 fueled** in fuel cell mode
  - **Vent gas recirculation** with purge
  - **Condenser** to remove water from H_2-side off-gas
  - Equipment models for **thermal management**
    - 1D multi-pass crossflow recuperative heat exchangers
    - 1D crossflow trim heaters



Block flow diagram of H_2–fueled SOC-based IES for Mode-Switching Operation

- Lee, A., et al.., J Adv Manuf Process 2021, 3(3) (2021).
- Bhattacharyya et al., Chem Eng Sci, 62, 4250-4267 (2007).
- Allan, D.A., et al., In Proc. FOCAPO/CPC (2023).

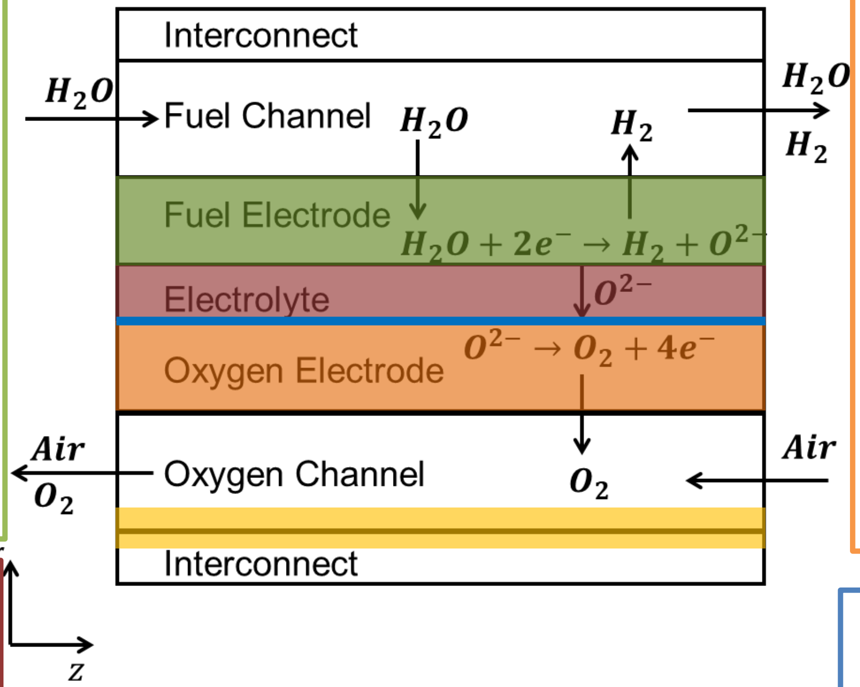
SOEC Microstructure Chemical Degradation Modeling

Fuel electrode nickel (Ni) agglomeration

- Ni particles grow with time under high temperature operation
- Ni_2OH formation drives the process
- Surface-diffusion – Ostwald ripening

$$\frac{d(d_{Ni})}{dt} = C \frac{X_{Ni}}{X_{YSZ} A_{YSZ} d_{Ni}^6} \left(\frac{Y_{H_2O}}{Y_{H_2}^{0.5}} \right) \exp\left(-\frac{E_a}{RT}\right)$$

Refs: J. Sehested et al. / *Applied Catalysis A*: General 309 (2006) 237–246



Lanthanum zirconate (LZO) scale growth

- At oxygen electrode under oxidizing conditions and high temperatures driven by high P_{O_2}

$$LaMnO_3 + ZrO_2 + 0.25O_2 \rightleftharpoons 0.5La_2Zr_2O_7 + MnO_2$$

- Parabolic growth law

$$\frac{dl_{LZO}(t)}{dt} = \frac{K_{g,LZO}}{2l_{LZO}(t) X_{0,LZO} \rho_{LZO}} exp\left(\frac{E_{LZO}}{RT}\right)$$

Refs: A. Kamkeng, and M. Wang. / *Chemical Engineering Journal* 429 (2022): 132158

YSZ electrolyte phase transformation

- Phase transformation of YSZ from cubic to tetragonal structure
- Results in decrease in electrolyte conductivity

$$\sigma_{El} = \sigma_{El,0}\left[\lambda + (1-\lambda)\exp\left(-\frac{t}{\tau}\right)\right]$$

Refs: Jiang et al. *Journal of the American Ceramic Society* 82(11):3057 - 3064

Chromium oxide scale growth

- Oxidation of chromium interconnect-oxygen electrode boundary
- Parabolic growth law

$$\frac{dl_{COS}(t)}{dt} = \frac{K_{g,COS}}{2l_{COS}(t) X_{0,COS} \rho_{COS}} exp\left(\frac{E_{COS}}{RT}\right)$$

Refs: D. Larrain et al. / *Journal of Power Sources* 161 (2006) 392–403

LSM-YSZ phase coarsening

- Driven by Mn^{2+} diffusion from LSM surface toward LSM-YSZ interface
- Results in loss of TPB length
- Model derived by assuming Fick's law diffusion of Mn^{2+}

$$\frac{L_{TPB}}{L_{TPB,0}} = 1 - 2 \times \left(\frac{t \times D_{LSM}}{\pi}\right)^{1/2}$$

Refs: A. Kamkeng, and M. Wang. / *Chemical Engineering Journal* 429 (2022): 132158

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Optimizing Long-Term SOEC System Operation

Case 1: Maximize Integral Efficiency

$$max \frac{1}{t_f - t_0} \int_{t_0}^{t_f} \eta_t dt$$

$st.$

$$h(x) = 0$$

$$\frac{dR}{dt} = f_R(x, t)$$

$$\eta_t = \frac{HHV(\dot{m}_{H_2,t})}{P_{in,total,t}} \qquad \forall t$$

Case 2: Minimize Final Degradation

$$min\, \Delta V \left(\widetilde{\theta_{t_f}}\right)$$

$st.$

$$h(x) = 0$$

$$\frac{dR}{dt} = f_R(x, t)$$

$$\theta_{tf} = \theta_{\ t0} + \int_{t_0}^{t_f} \dot{\theta}(x, \theta) dt$$

Decision variables at each time point:

1. Feed heater duties
2. Sweep heater duties
3. Sweep blower flowrate
4. Feed exchanger flowrate
5. Feed recycle ratio
6. Sweep recycle ratio

Case 3: Minimize Levelized Cost of Hydrogen (LCOH)

$$LCOH = \frac{CRF_{BOP} CC_{BOP} + \sum_{i=1}^{R} CRF_{stack,i} CC_{stack} + OC + EC}{m_{H_2,\text{lifetime}}}$$

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Quasi-Steady State Optimization Results for 3 Objective Functions under Galvanostatic, Potentiostatic, and Flexible Operation for Low- and High-Price Electricity Markets

		Electricity Price = 0.03 \$/kWh		Electricity Price = 0.3 \$/kWh	
Operating Profile	Objective Function	Replacement Schedule (years)	LCOH (\$/kg H_2)	Replacement Schedule (years)	LCOH (\$/kg H_2)
Galvanostatic Operation	Minimize terminal degradation	5	2.00	5	13.00
	Maximize Integral Efficiency	2	2.29	2	11.92
	Minimize LCOH	5	1.93	2.5	11.84
Potentiostatic Operation	Minimize terminal degradation	3	2.11	3	12.51
	Maximize Integral Efficiency	2	2.30	2.0	11.93
	Minimize LCOH	3	2.05	2.0	11.91
Free Operation	Minimize terminal degradation	5	1.99	5	13.01
	Maximize Integral Efficiency	3	2.02	2.5	11.78
	Minimize LCOH	5	1.92	2.5	11.78

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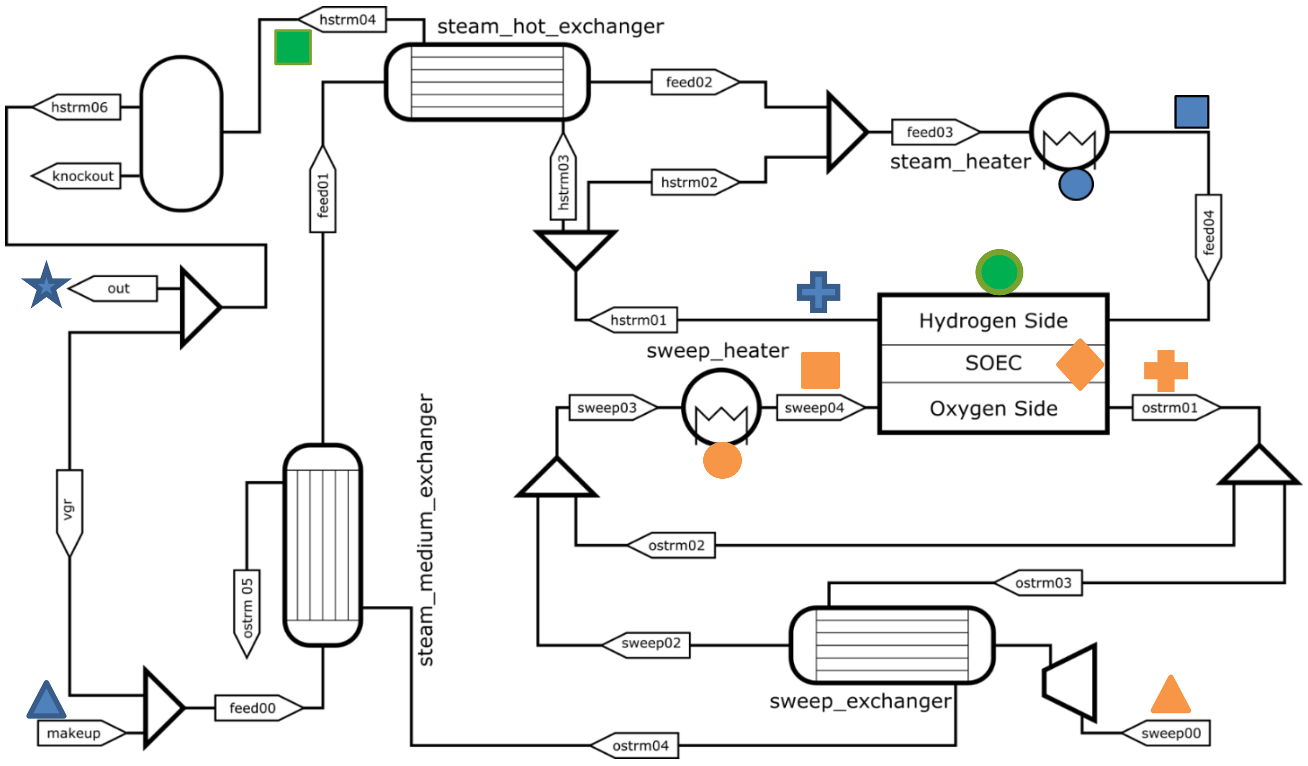
Process Control for SOC-based System Mode-Switching

- **Classical Control: Proportional-Integral-Derivative (PID)**
- **Nonlinear Model Predictive Control (NMPC)**
  - Well-suited to highly interactive manipulated variables and constraint handling



Controller	Manipulated Variables (MVs)	Controlled Variables (CVs)
PID, NMPC	Cell potential	Outlet Water Concentration
PID, NMPC	Steam/H_2 feed rate	H_2 production rate
PID, NMPC	Feed heater duty	Feed heater outlet temperature
PID, NMPC	Sweep heater duty	Sweep heater outlet temperature
PID, NMPC	Steam heater outlet temperature setpoint*	SOC steam outlet temperature
PID, NMPC	Sweep heater outlet temperature setpoint*	SOC sweep outlet temperature
PID, NMPC	Sweep feed rate	SOC temperature
NMPC	Feed recycle ratio	
NMPC	Sweep recycle ratio	
NMPC	Vent gas recirculation (VGR) recycle ratio	
NMPC	H_2/H_2O ratio in make-up	

**artificial control variables*

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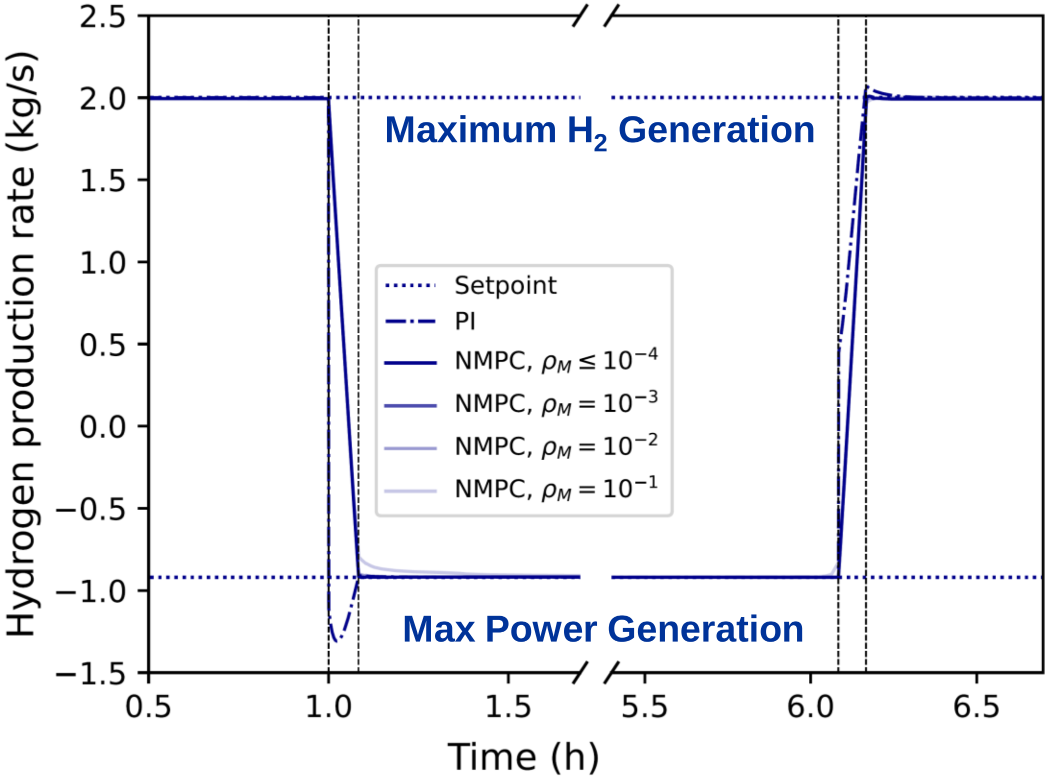
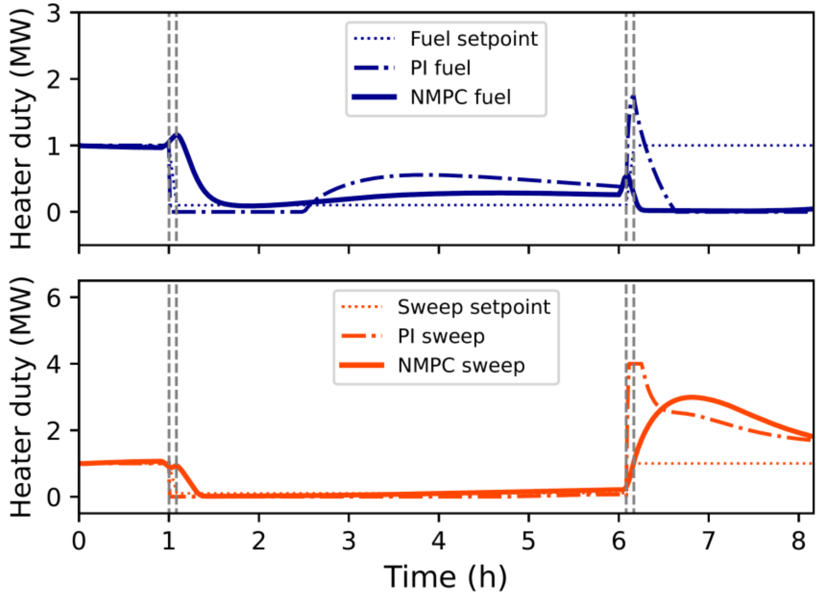
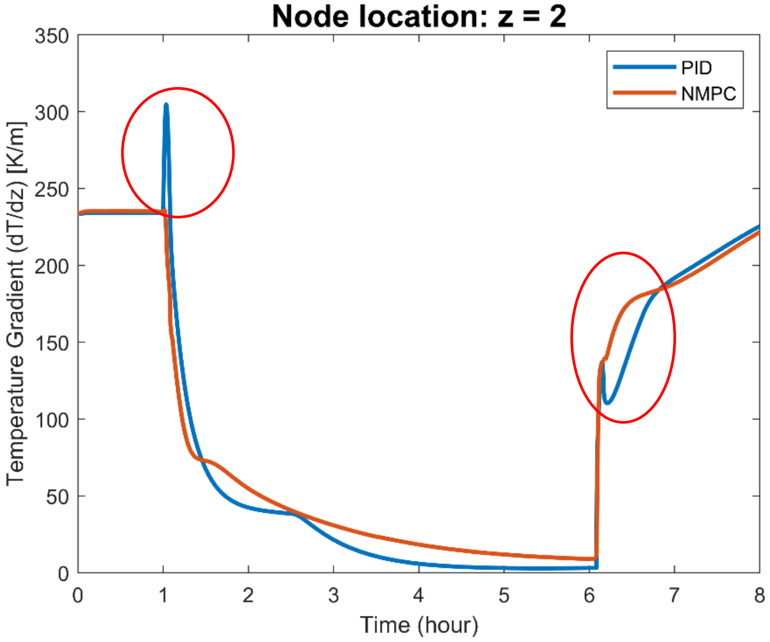
- Allan, D.A., et al., In Proc. FOCAPO/CPC (2023).
- Dabadghao, V., Ph.D. Thesis, CMU (2023).

Dynamic Simulation and Control Results for Ramping Operation







- **Classical PI control** of H_2 production rate shows **overshoot**, not exhibited by NMPC
- **NMPC** yields **smoother heater duty profiles** than PI control
- **NMPC** yields **smoother SOC temperature gradient** and lower spatial extremum magnitude than PI control

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Summary

- IDAES has become a foundational modeling and optimization platform enabling us to address several major national and DOE priorities.

- The core program is focused on ensuring existing projects leveraging IDAES are successful while continuing to build out new capabilities.
  - Integrating short-term operational realities into long term expansion planning of reliable, decarbonized grids.
  - Integrating manufacturing considerations into process design to reduce both deployment times & manufacturing costs.
  - Optimizing the design, operation, and control of integrated power and H_2 systems.

- Several advanced dynamic optimization & control capabilities have been recently developed for flexible SOC systems.
  - Long-term SOEC optimization considering chemical degradation can be used to optimize stack replacement schedule and operating trajectories.
  - Nonlinear model predictive control (NMPC) can explicitly restrict temperature gradients/curvatures or other constraints compared to classical control.

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