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Institute for the Design of Advanced Energy Systems

Institute for the Design of Advanced Energy Systems

Anthony Burgard, Carl Laird

October 11th, 2023

NATIONAL ENERGY TECHNOLOGY LABORATORY
BERKELEY LAB
Sandia National Laboratories
Carnegie Mellon
West Virginia University
UNIVERSITY OF NOTRE DAME
Georgia Tech
U.S. DEPARTMENT OF ENERGY

Objective of Core IDAES Program

- IDAES enables the design and optimization of the increasingly **integrated** and **dynamic** energy and process systems of the future with an emphasis on facilitating deep decarbonization of the energy and industrial sectors.

- Major Focus Areas

  1. Continue to build out advanced capabilities
  2. Grow the user base in strategic areas
  3. Ensure that existing projects leveraging IDAES are successful !!!

Foundational Modeling and Optimization Partnerships Utilizing IDAES

Multi-lab Initiatives to Address Major National and DOE Priorities

Initiative	Focus	Partners
IDAES (Institute for the Design of Advanced Energy Systems)	H_2 with Capture	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	National Energy Technology Laboratory, Berkeley Lab, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Pacific Northwest National Laboratory, Oak Ridge National Laboratory, Carnegie Mellon, West Virginia University, University of Notre Dame, The University of Texas at Austin, UT, University of Pittsburgh
DISPATCHES (Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems)	Hybrid Energy Systems	National Energy Technology Laboratory, Sandia National Laboratories, Berkeley Lab, Idaho National Laboratory, NREL Transforming ENERGY, University of Notre Dame
Water TAP	Water Desalination	National Energy Technology Laboratory, Berkeley Lab, NREL Transforming ENERGY, Oak Ridge National Laboratory
PrOMMiS	Rare Earth Element & Critical Mineral Recovery	National Energy Technology Laboratory, Berkeley Lab, Sandia National Laboratories, Carnegie Mellon, West Virginia University, University of Notre Dame, Georgia Tech
PARETO (The Produced Water Optimization Initiative)	Produced Water Management	National Energy Technology Laboratory, Berkeley Lab, Carnegie Mellon, Georgia Tech

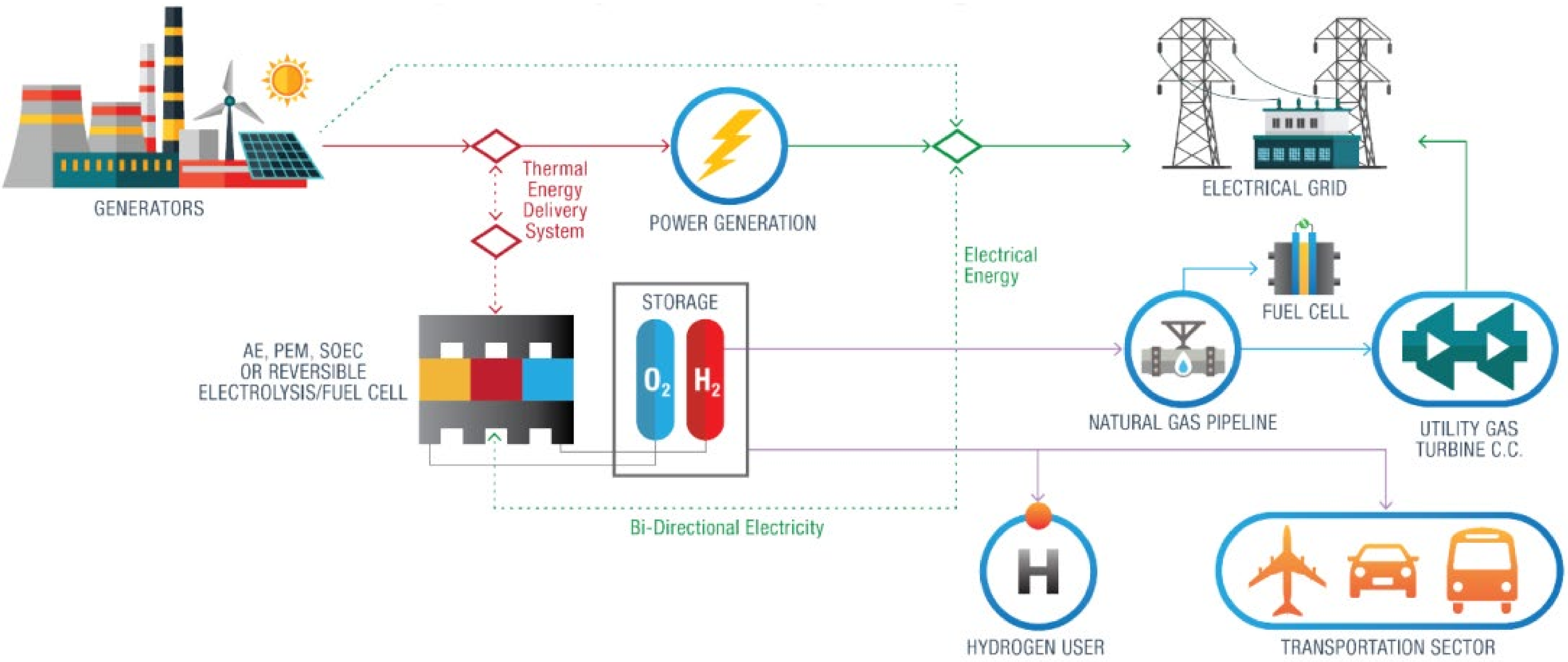
IDAES-Core Now Supported by FECM's Hydrogen with Carbon Management Program

- **Objective:** Develop clean hydrogen as a cost-competitive alternative base fuel for power generation, energy storage and industrial heat.
- Reduce H_2 costs of $1/kg within one decade (1-1-1) with life cycle GHG emissions reductions (including from methane) of 90% vs current levels.
- Current application areas:
  - Point source capture from gasification and reforming
  - Modular co-gasification of waste plastics (or MSW), biomass, and waste coal
  - Reversible solid oxide fuel cells
  - Hydrogen turbines
  - Clean hydrogen hubs

IDAES New Capability Development

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

Integrated Energy System for Low Carbon Power and H_2



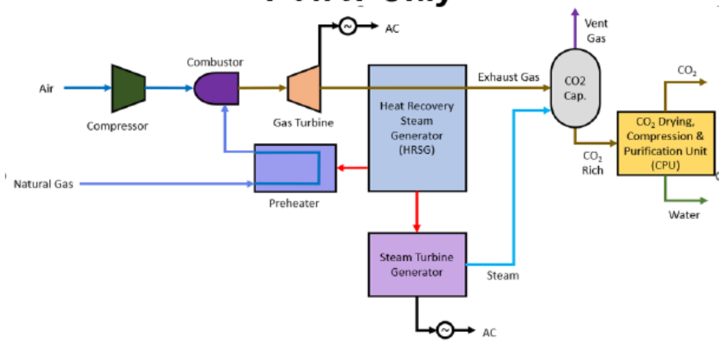
The IDAES platform is being applied to explore whether tightly coupled integrated energy systems that have the flexibility to produce both power and hydrogen should play a role in DOE's goals of decarbonizing the power sector by 2035 and broader economy by 2050.

Analysis of Integrated Energy System Concepts

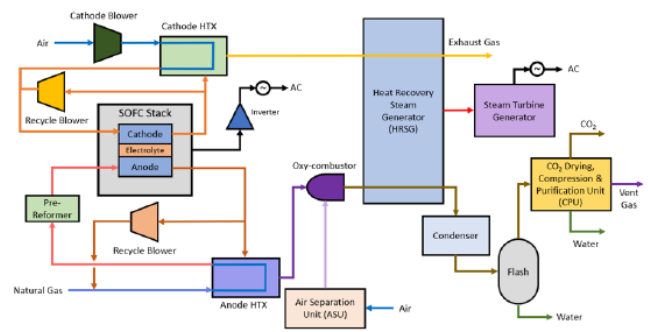
Fuel = Natural Gas
CO_2 capture > 97%

Baseline Systems Single Product

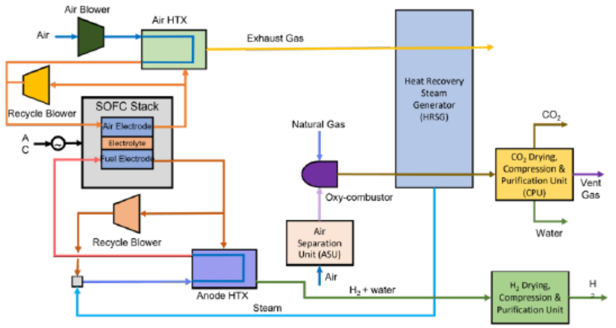
Standalone Natural Gas Combined Cycle (NGCC)
Power Only



Standalone Solid Oxide Fuel Cell (SOFC)
Power Only

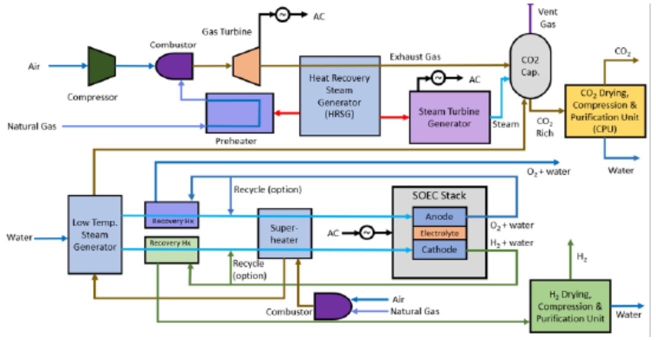


Standalone Solid Oxide Electrolyzer Cell (SOEC)
Hydrogen Only

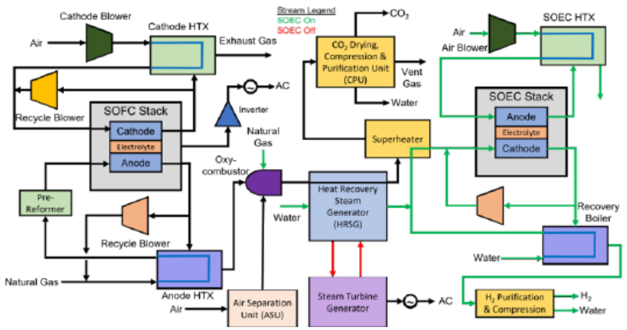


Integrated Systems Multi-Product

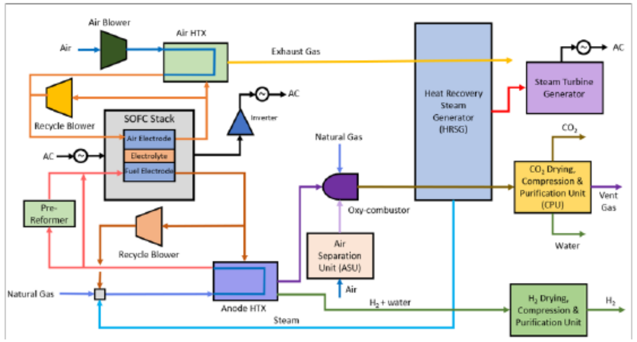
NGCC + SOEC
Power, Hydrogen, Coproduction



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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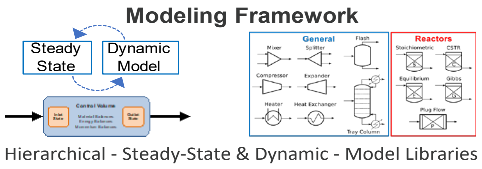
Process Concept Evaluation Strategy

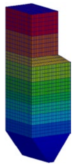
Develop process and costing models using IDAES that are capable of optimization and off-design performance prediction



Calculate standard metrics like

- **$/MWh**
- **$/kg H_2**
- **kg $CO2_{eq}$/MWh**
- **kg $CO2_{eq}$/kg H_2**

AI/ML
Surrogate Modeling



Develop surrogate models for each process concept that relate variable costs with power and H_2 output (and fixed costs with power and H_2 capacities)

Use surrogate models in **multi-period process/market optimization model** to calculate optimal **capacity factors** and **net profit** under several scenarios.

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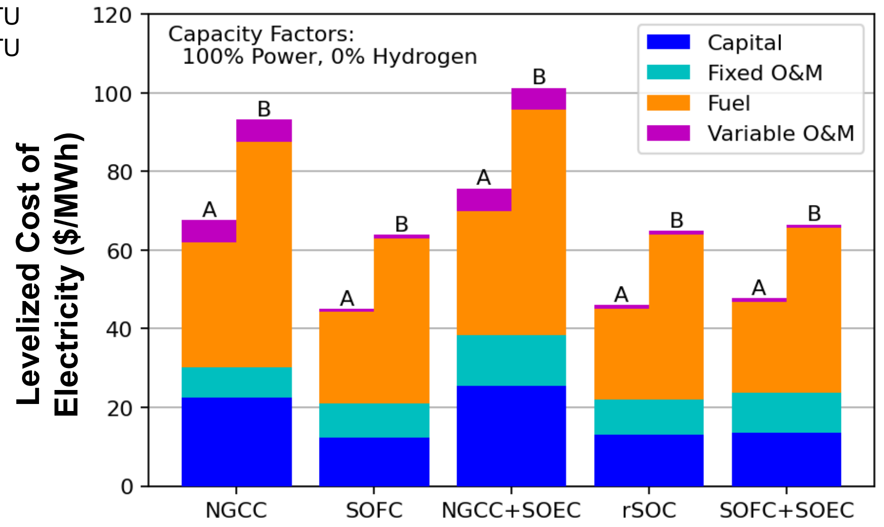
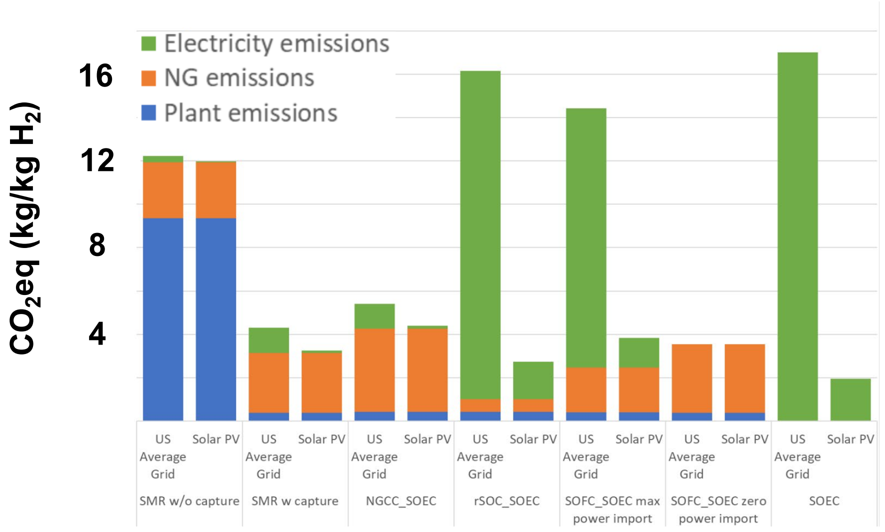
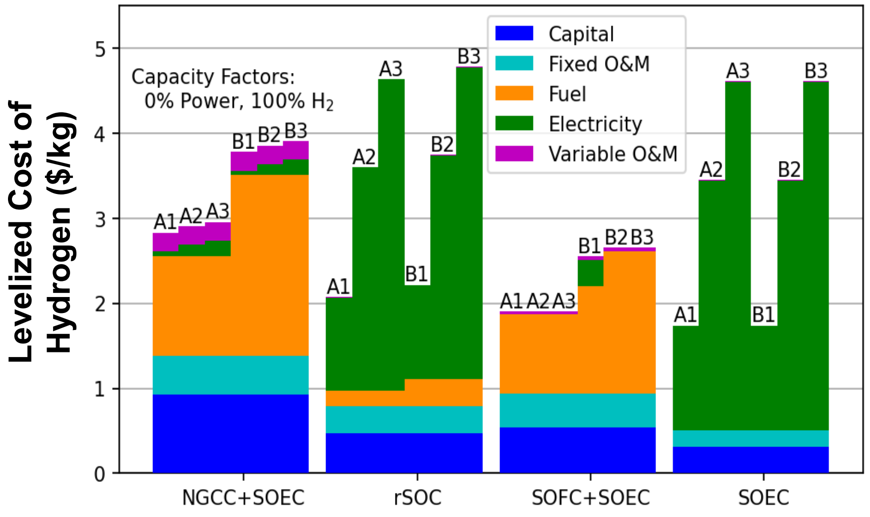
Conventional Process-Centric Analysis was Rigorous but Limited

A = $4.42 / mmBTU
B = $8.00 / mmBTU
1 = $30 / MWh
2 = $71.7 / MWh
3 = $100 / MWh







- Lowest cost system highly dependent on many factors (NG, H_2, electricity prices, CO_2 incentives or taxes)
- A different analysis approach is required to more fully understand the value proposition of such systems.

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Eslick, Noring, Susarla, Okoli, Allan, Wang, Ma, Zamarripa, Iyengar, Burgard, Technoeconomic Evaluation of Solid Oxide Fuel Cell Hydrogen-Electricity Co-generation Concepts (DOE/NETL-2023/4322).

Multi-Period Optimization, Price-Taker Assumption*

Input: Electricity prices for a given market

Input: H_2 Selling Price

Output: Power and H_2 generated at every time step

For now, just assume that capacities, P_{max} and H_{max}, are fixed

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

s.t.

$$p_t \leq P_{max}\ \forall t \in T$$

$$h_t \leq H_{max}\ \forall t \in T$$

Extensions not shown:

- Buying electricity from grid
- Price of NG on variable costs
- Carbon taxes
- Ramping constraints
- Start up shutdown costs

Disjunctions at every time step to choose optimal operating mode:

$$\begin{bmatrix} C_{var}(p_t, h_t) = 0 \\ p_t = 0 \\ h_t = 0 \\ \ \end{bmatrix} \veebar \begin{bmatrix} C_{var}(p_t, h_t) = f_1(p_t) \\ p_t \geq P_{min} \\ h_t = 0 \\ p_t^h = 0 \end{bmatrix} \veebar \begin{bmatrix} C_{var}(p_t, h_t) = f_2(h_t) \\ h_t \geq H_{min} \\ p_t^h = f_4(h_t) \end{bmatrix} \veebar \begin{bmatrix} C_{var}(p_t, h_t) = f_3(p_t, h_t) \\ p_t^h = f_5(h_t) \\ p_t \geq P_{min} \\ h_t \geq H_{min} \end{bmatrix}$$

Plant is off | Power only | Hydrogen only | Both Power and Hydrogen

More advanced formulations:
Presentation (this afternoon):
Advances in Modeling Power Generation Grid and Market Interactions (DISPATCHES) Alex Dowling, John Siirola

Poster:
Multi-scale Optimization of Integrated Energy Systems that Co-Produce Electricity and Hydrogen Using Market Surrogates
Xinhe Chen

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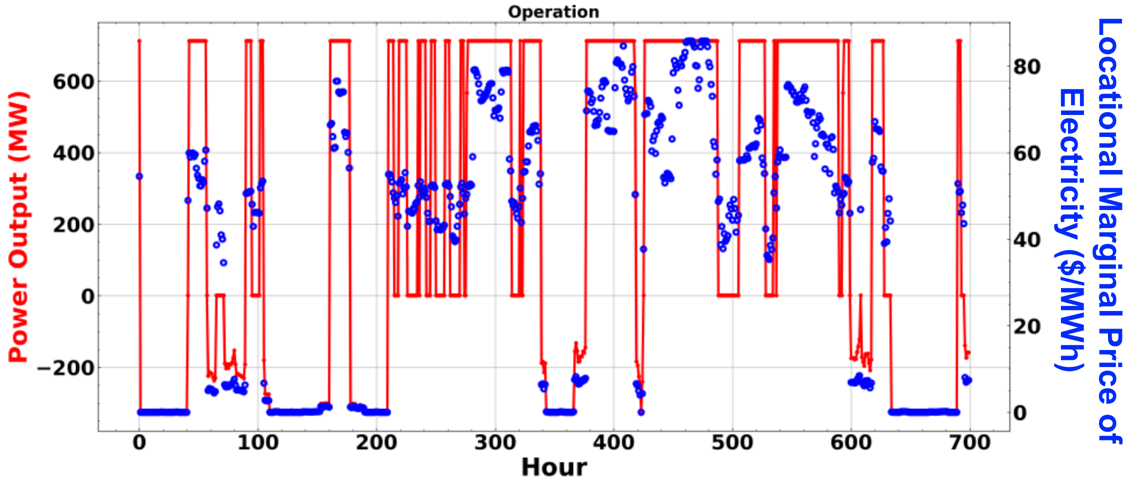
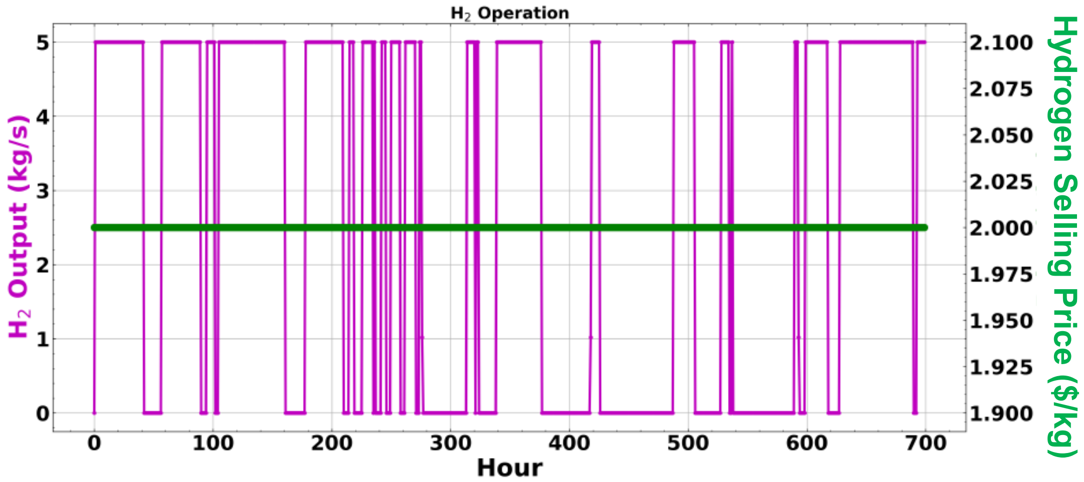
Many Electricity Market Scenarios Considered

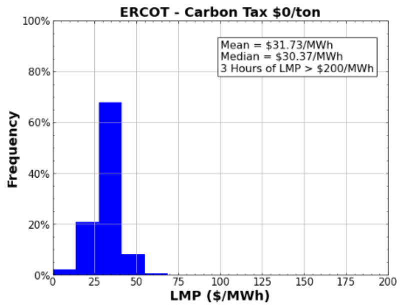
- **61 total data sets** (every hour for a year)
- 2019 & 2022 data from ERCOT, ISO_NE, MISO, PJM, SPP, NYISO
- Future projections from NREL and Princeton from ARPA-E FLECCS program
- Future projections from NETL for ERCOT using PROMOD IV

System: SOFC + SOEC
Scenario: MiNg_$100_MISO-W_2035 (only first 700 hours of year shown)

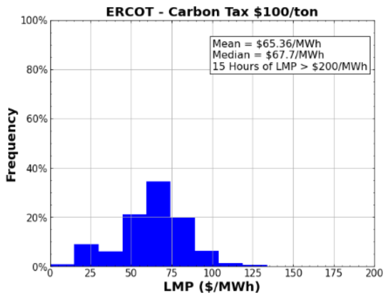




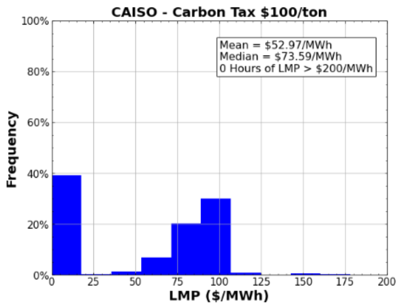
Data sets cover very broad range of potential scenarios



Low Prices



High Prices



Bimodal (e.g., high VRE)

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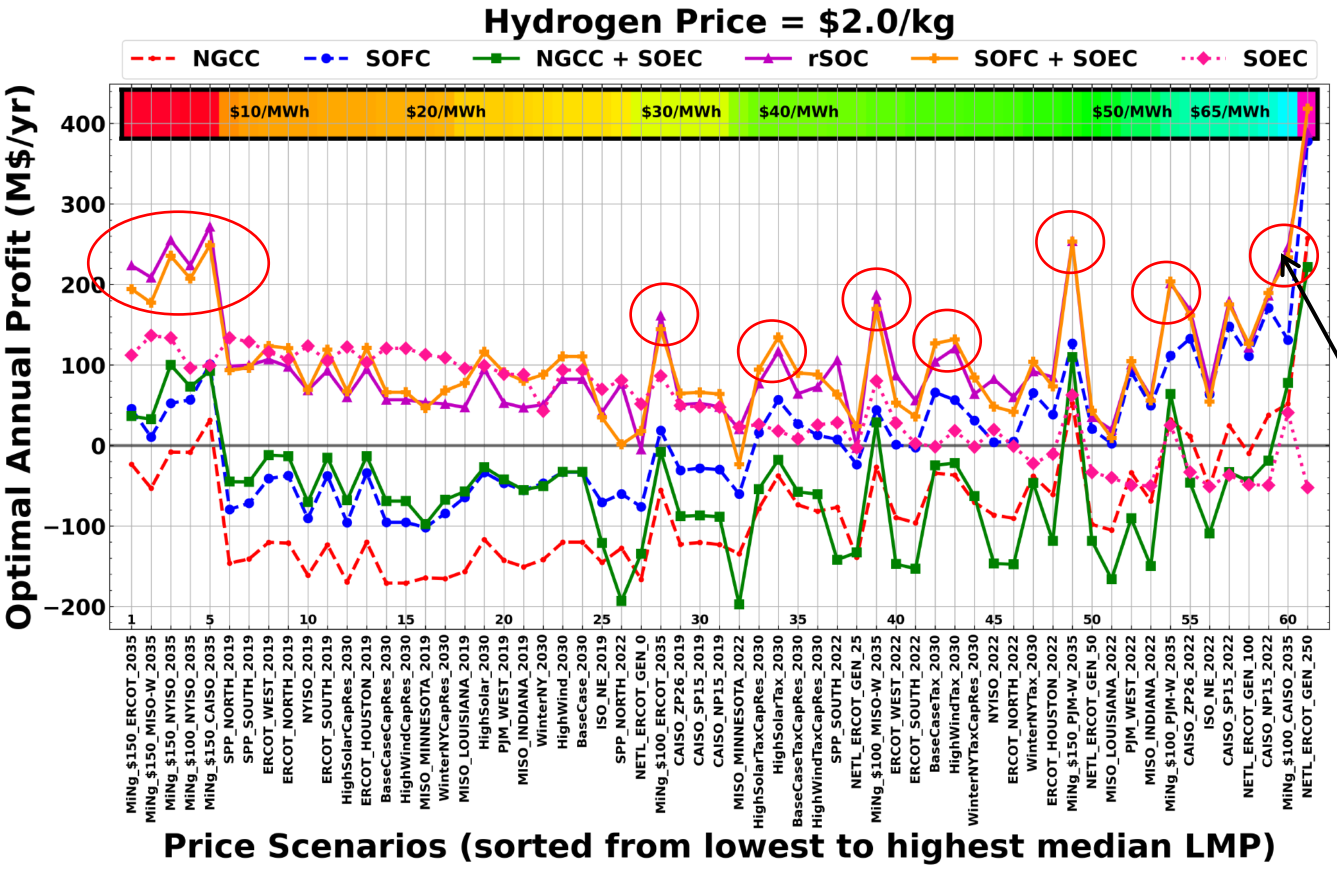
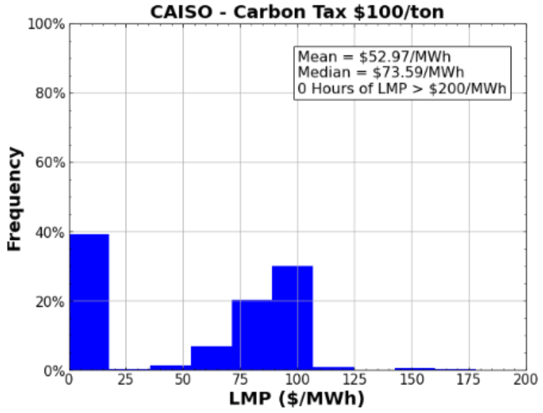
Compiled Results from Integrated Process/Market Optimization



% 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.



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

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Take Home Messages

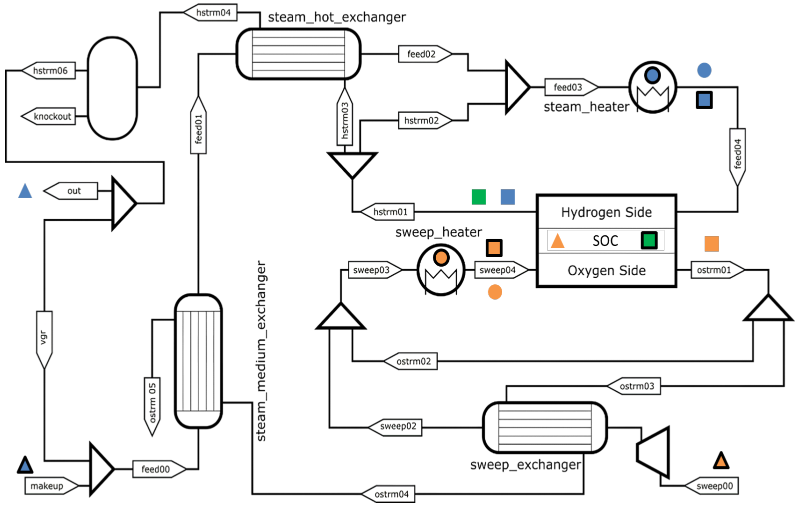
- The IDAES platform enabled rigorous comparisons of processes across diverse market scenarios leading to insights beyond conventional TEA.

- This is perhaps the first study to quantitatively make the business case for why DOE is investing in reversible SOFC technology.

- Emphasis in 2023 on developing publicly available, configurable, workflow for process/market optimization that reduces analysis time from months to weeks.
  - Flexible carbon capture
  - Hybrid energy systems (e.g., nuclear, solar, fossil + capture)
  - Integrated DAC systems

Integrated Dynamic H_2 and Power Systems

- **Research Challenge**
  - SOC-based systems need to operate flexibly with fluctuations in electricity prices.
  - How can one best operate and control SOC-based systems for mode-switching (H_2/power), while minimizing degradation over long-term operation?
- **Key Findings**
  - Nonlinear model predictive control (NMPC) can track H_2 and power production setpoints, while mitigating SOC temperature gradients and mixed partial derivatives during mode-switching.
  - Long-term performance/degradation optimizations (20K hours) show that choice of optimal operational scenario depends on tradeoff between energy costs and SOC replacement costs.



SOC system for H_2 and power production

See also:

Oct 12, General Session, AM
Making Models Dynamic and Controllable
Doug Allan

Posters
NMPC for Mode-Switching Operation of Reversible Solid Oxide Cell Systems
Doug Allan, Michael Li

Optimal Long-Term Operation of Solid Oxide Electrolyzers considering Physical and Chemical Degradation
Nishant Giridhar

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IDAES New Capability Development

- Integrated process market optimization of power and H_2 systems
- Dynamics, control, health modeling and optimization of power and H_2 systems
- **Integrating manufacturing considerations into process design**
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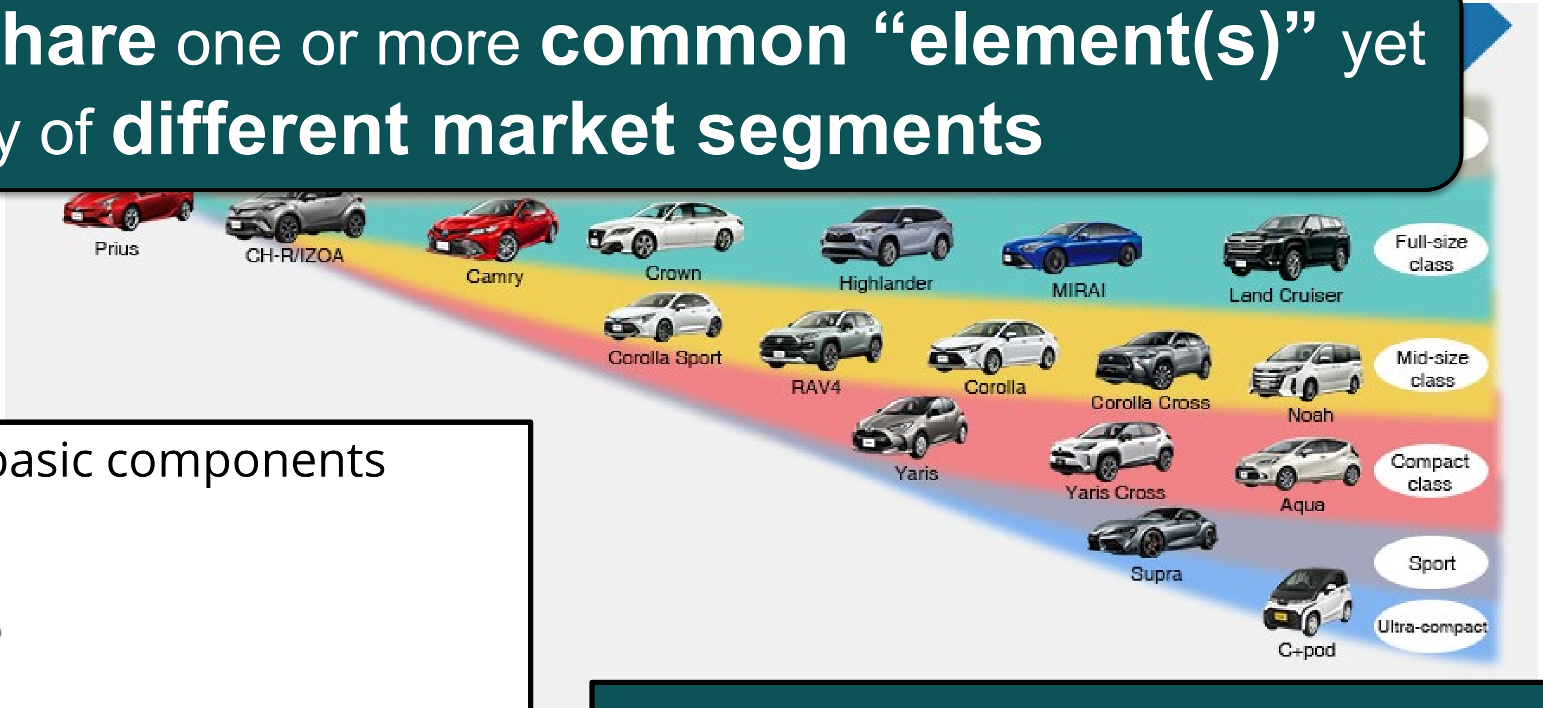
Product Family and Platform Design

A **set of products** that **share** one or more **common “element(s)”** yet target a variety of **different market segments**

these car models



- Each vehicle shares a combination of basic components
  - Steering, interior seats, frame, etc.

Complete optimization on basic areas

- The rest is customized to a specific model
  - Appearance, engine (Toyota uses another platform for this), etc.

Focus on each car type

Toyota builds 70% of cars on this platform

- 20% reduction in manufacturing cost
- Increased competitiveness + flexibility
- Reduced investment for product develop.

https://global.toyota/en/mobility/tnga/
https://global.toyota/en/mobility/tnga/powertrain2018/feature/
https://global.toyota/pages/global_toyota/ir/financial-results/2019_1q_competitiveness_en.pdf

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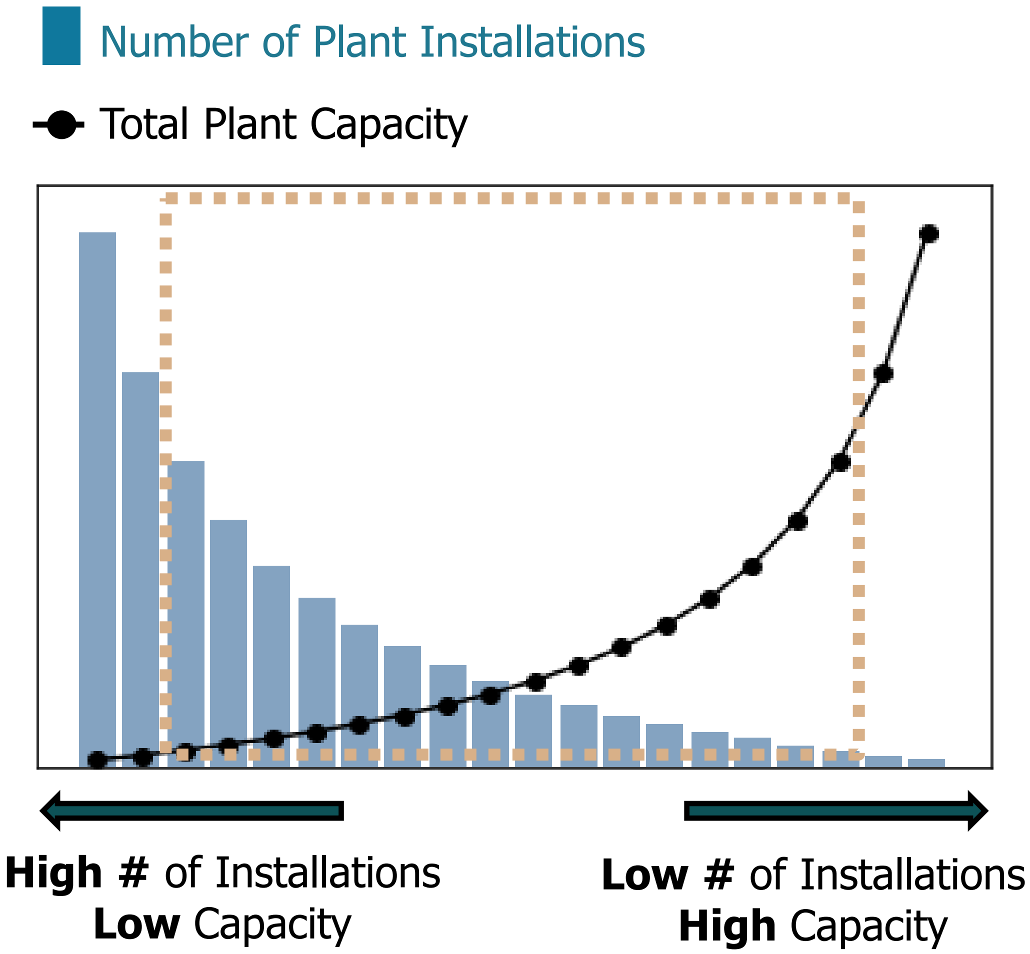
Background



Climate change goals require **rapid, broad** deployment of new technologies and process variants for different applications

- Reduce time to deployment through decreased engineering design effort
  - Avoid unique and independent designs for each installation
- Improve manufacturing timelines and costs
  - Exploit economies of numbers
  - Reduce manufacturing complexity
- Simultaneous platform and process design
  - Assemble processes from a smaller subset of subcomponents (platform)

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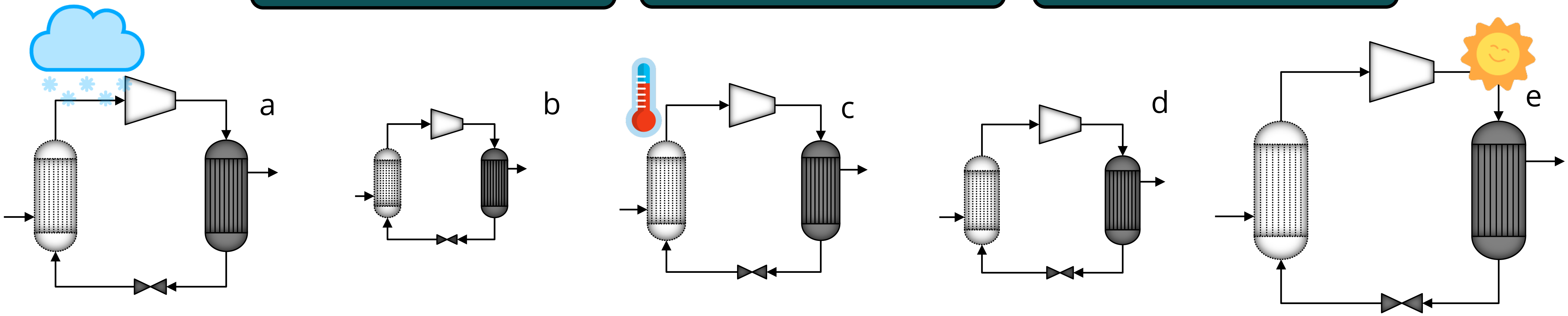
Mapping to PSE: Process Family Design

Variations could be from:

design requirements

environmental conditions

capacity



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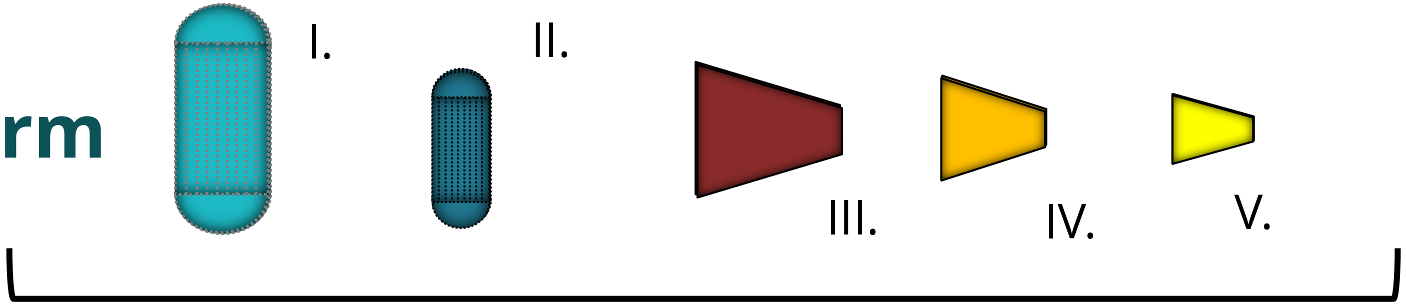
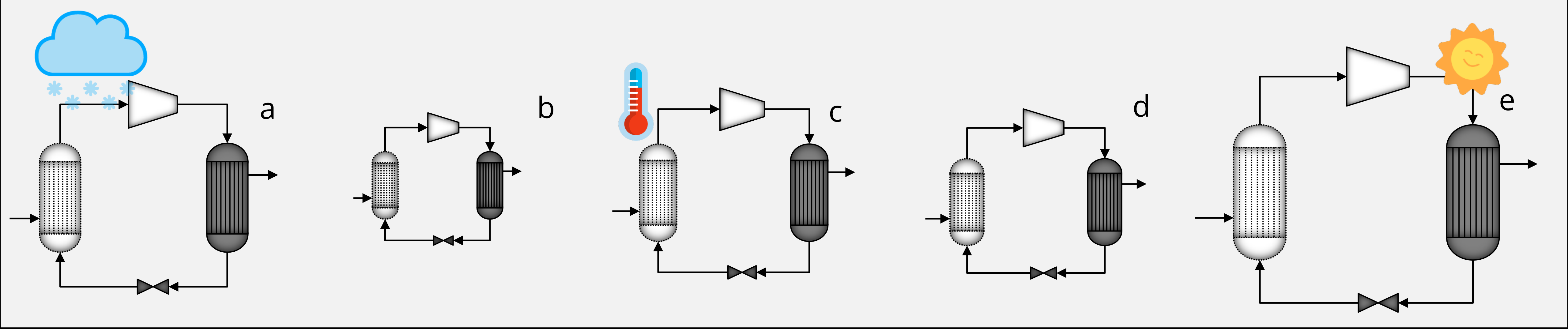
Mapping to PSE: Process Family Design

Process Platform





Process Family

Optimization Formulation

$v \in V$	set of process variants
w_v	parameter weight of each process variant v
p_v	variable cost of each process variant v
$m \in M$	set of unit module types
$\mathbf{r}_v$	parameter vector of design requirements for variant v
$\mathbf{d}_{v,m}$	variable vector unit module design of unit module type m for variant v
$\mathbf{o}_v$	variable vector of operating variables for all $m \in M$ for variant v
$\mathbf{i}_v$	variable vector of performance indicators for process variant v
$c \in C$	set of *common* unit module types ($C \subseteq M$)
$l \in L_c$	set labels for all designs of common unit module types $c \in C$
$\hat{\mathbf{d}}_{c,l}$	variable vector describing l-labeled unit module design for unit module c
$\mathrm{Y}_{v,c,l}$	decision variable; selection of common unit module designs

$$\text{min.} \quad \sum_{v \in V} w_v p_v$$

s.t.

$$p_v = f_v^p(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}, \mathbf{o}_v) \qquad \forall\, v \in V$$

$$\mathbf{i}_v = f_v^i(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}, \mathbf{o}_v) \qquad \forall\, v \in V$$

$$0 = h(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}, \mathbf{o}_v) \qquad \forall\, v \in V$$

$$\underset{l \in L_c}{\veebar} \begin{bmatrix} \mathrm{Y}_{v,c,l} \\ \mathbf{d}_{v,c} = \hat{\mathbf{d}}_{c,l} \end{bmatrix} \qquad \forall\, v \in V, c \in C$$

$$\hat{\mathbf{d}}_c^{\mathrm{LB}} \le \hat{\mathbf{d}}_{c,l} \le \hat{\mathbf{d}}_c^{\mathrm{UB}} \qquad \forall\, c \in C, l \in L_c$$

$$\mathbf{o}_v^{\mathrm{LB}} \le \mathbf{o}_v \le \mathbf{o}_v^{\mathrm{UB}} \qquad \forall\, v \in V$$

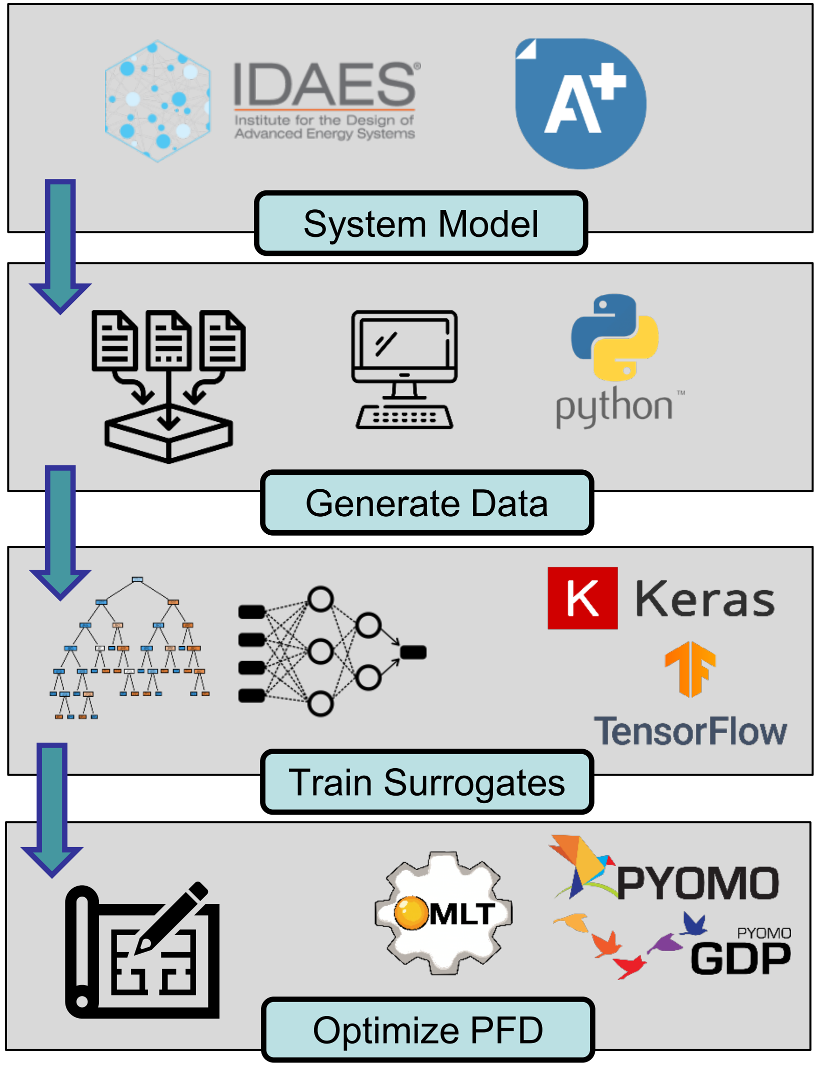
$$\mathbf{i}_v^{\mathrm{LB}} \le \mathbf{i}_v \le \mathbf{i}_v^{\mathrm{UB}} \qquad \forall\, v \in V$$

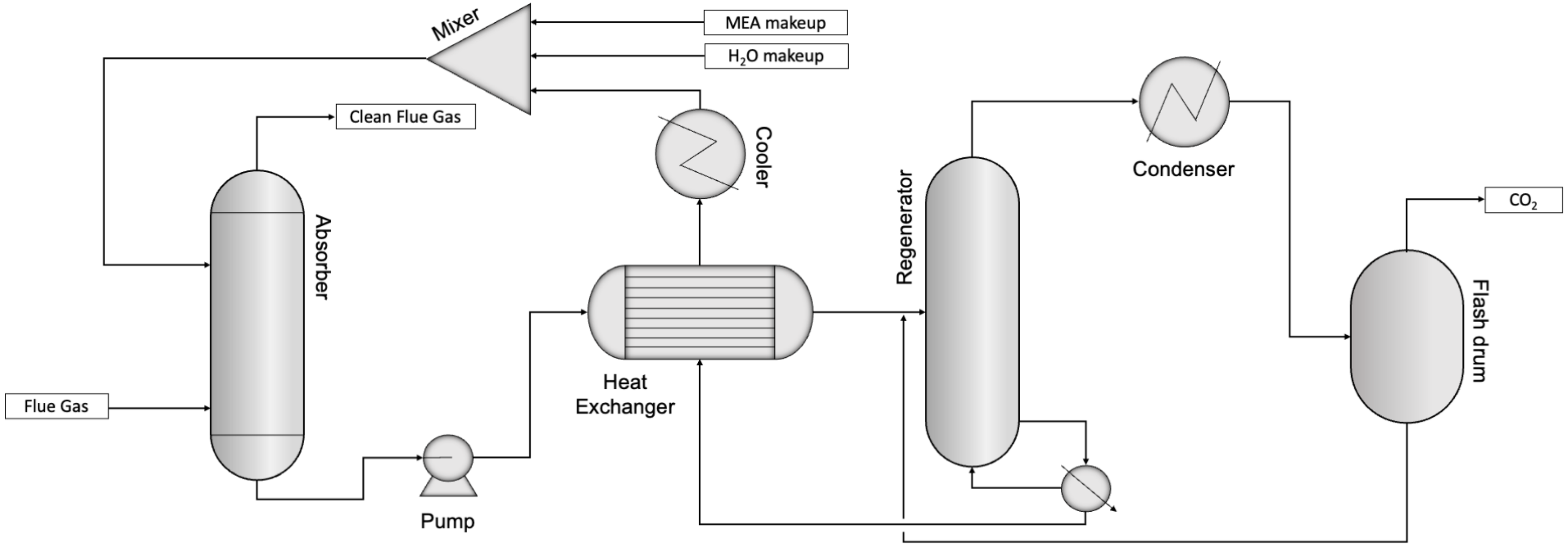
$$\mathrm{Y}_{v,c,l} \in \{\text{True}, \text{False}\} \qquad \forall\, v \in V, c \in C, l \in L_c$$

Several different formulations based on this foundation

- Discretization → MILP
- Use of ML surrogates → MILP
- Direct solution of MINLP

Computational Framework for MEA Process Family Design





CO_2 Rich Gas Flow Rate

Flue Gas Flow Rate Range
2,000 kg/hr – 3,000 kg/hr

CO_2 Rich Gas Conc.

Flue Gas CO_2 Concentration Range
0.1 – 0.25 (mass fraction)

Range of conditions (concentrations) from NGCC → industrial applications

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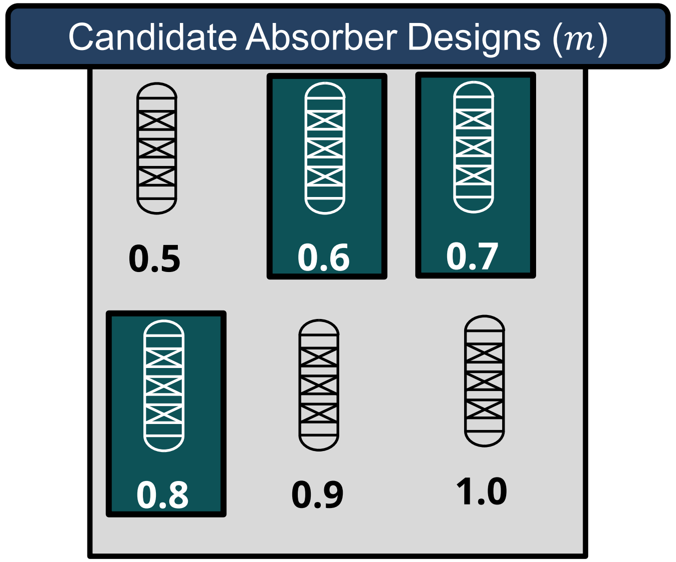
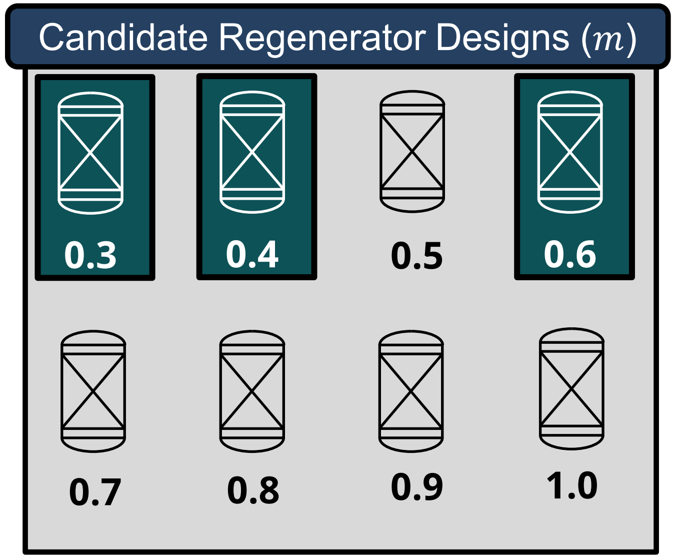
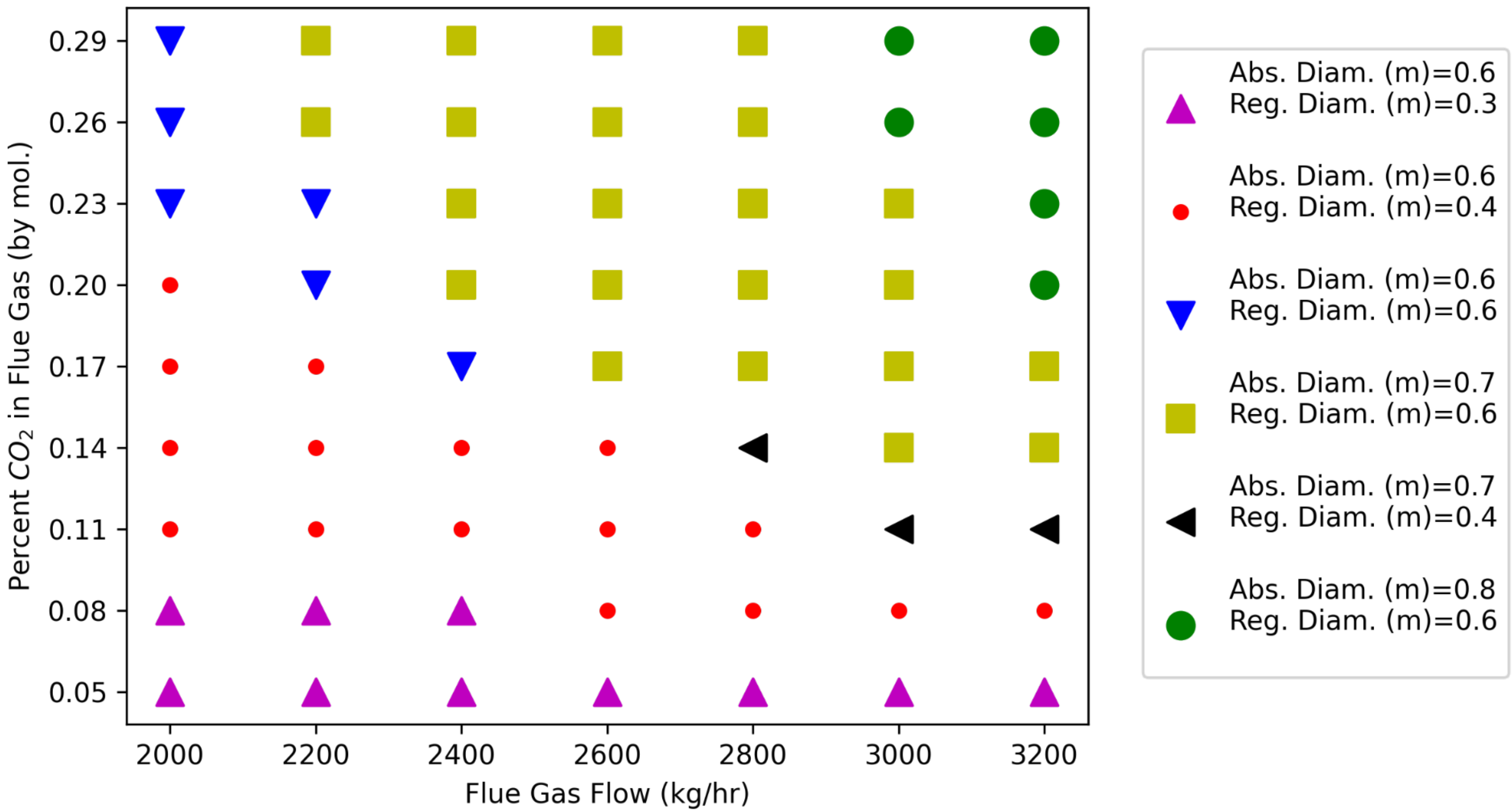
Discretization Formulation
Case Study 2: MEA Carbon Capture







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Conclusions and Current Work

- Process family design: alternative to build-to-order & pure modularity
- Reduced costs and time to deployment
  - Modular concepts at unit level → economies of numbers
  - Customization to the design range → economies of scale
  - Reduced engineering design time/effort
  - Reduced manufacturing time/costs
- Multiple scalable optimization formulations
- **Estimated capital cost reductions of 8-14% (using literature parameters)**

Current Work

- Incorporate economies of numbers within optimization formulation
- Decomposition strategies for larger-scale problems: Alg. → HPC
- Extensions to other climate change processes

IDAES New Capability Development

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- Dynamics, control, health modeling and optimization of power and H_2 systems
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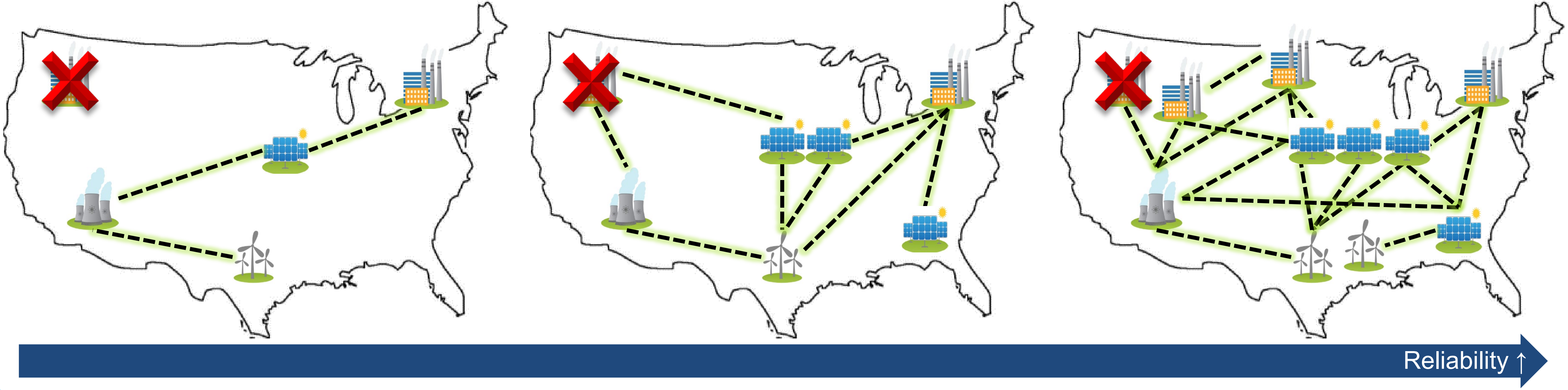
Infrastructure Planning of Reliable & Carbon-Neutral Power Systems

- **Objective**
  - To determine long-term (yearly) investment decisions for future carbon-neutral power systems 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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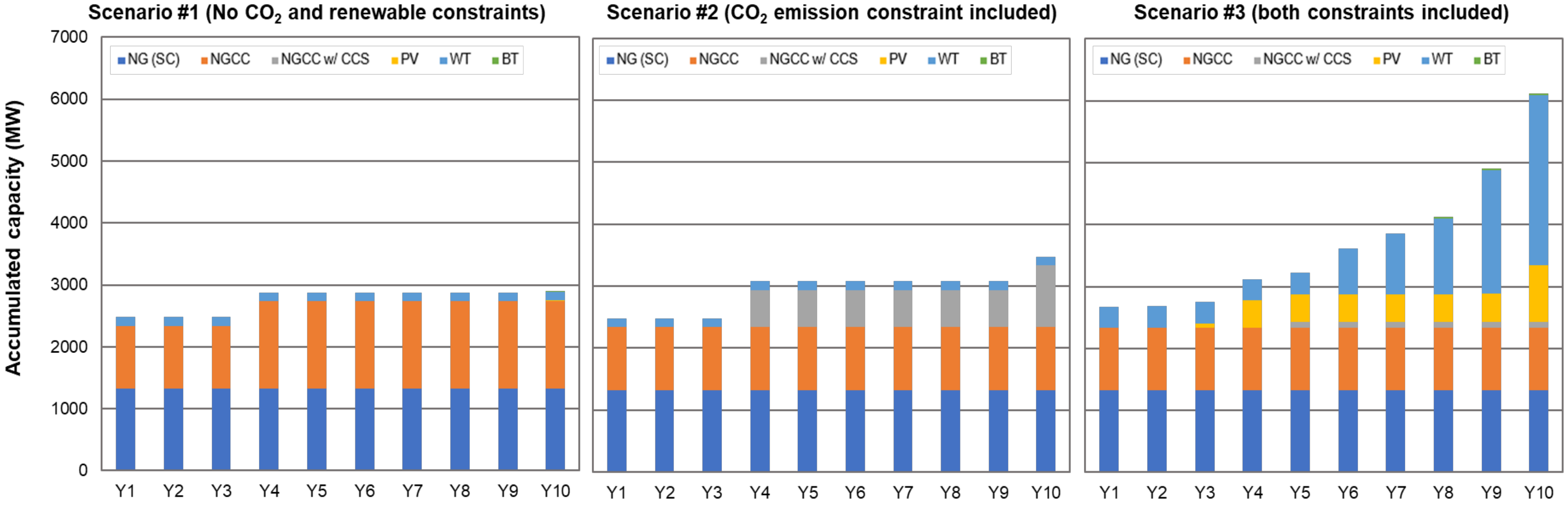
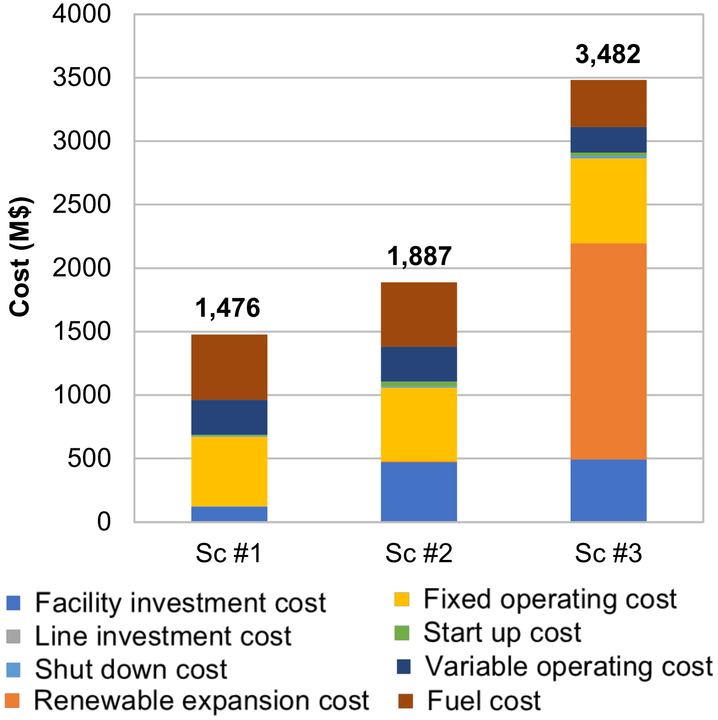
Infrastructure Planning of Reliable & Carbon-Neutral Power Systems

- **San Diego County Case Study**

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





See also:

Presentation (this afternoon)

Advancing the State of the Art in Expansion Planning for the California Grid in Partnership with IDAES

Seolhee Cho, Chris McLean, Ben Omell

Posters

Optimization for Infrastructure Planning of Reliable and Carbon-neutral Power Systems: Application to San Diego County

Seolhee Cho

Flexible Modular Formulations for Grid Infrastructure Planning

Kyle Skolfield

ML-Guided Optimization of Energy Systems

Nick Sahinidis

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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 advanced capabilities.
  - Examining the design, market potential, dynamics, and controllability of integrated power and H_2 systems.
  - Explicitly integrating manufacturing considerations into process design to reduce both deployment times and manufacturing costs.
  - Better integrating short-term operational realities into long term expansion planning of reliable, decarbonized electricity grids.
- Emphasis in 2023 on developing diagnostics and enhanced visualization features a direct result on stakeholder feedback.

Acknowledgements

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2023 Joint CCSI$_2$/IDAES Technical Team Meeting
Lawrence Berkeley National Lab

https://idaes.org/about/contact-us/

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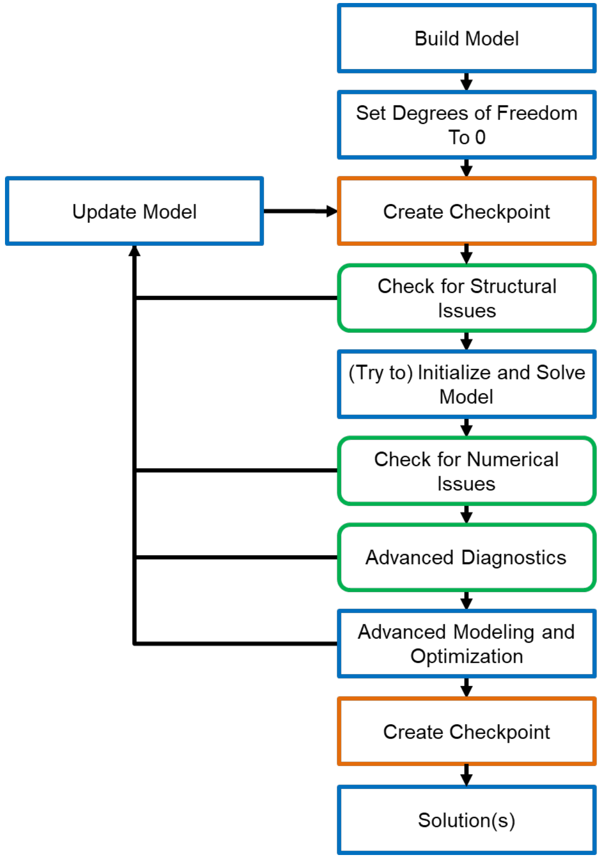
Diagnostics and Visualization



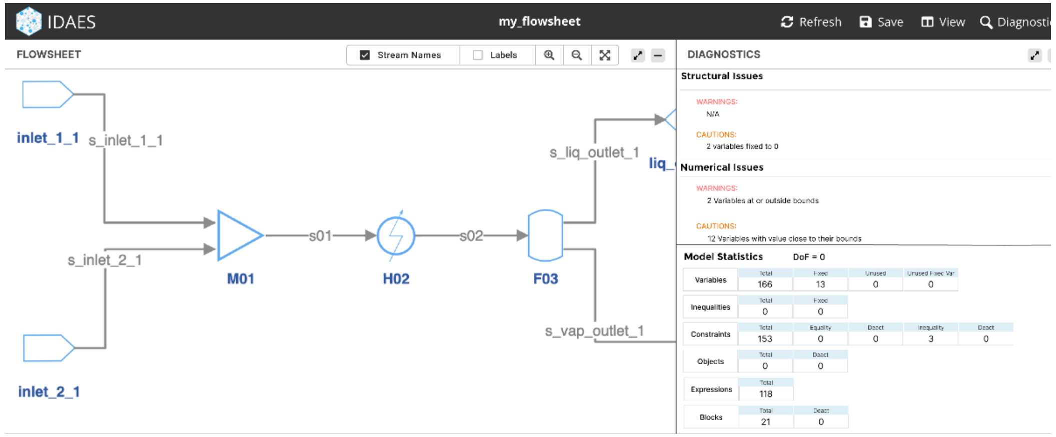
- **Research Challenge**
  - Solving EO models is extremely challenging, and often takes significantly more time than initial model development.
  - Despite decades of experience, there are no published workflows for debugging models
- **Objectives**
  - Develop tools and workflows for model diagnostics to assist users with developing and troubleshooting models.
  - Make diagnostic information visually accessible to model developers.

See also:

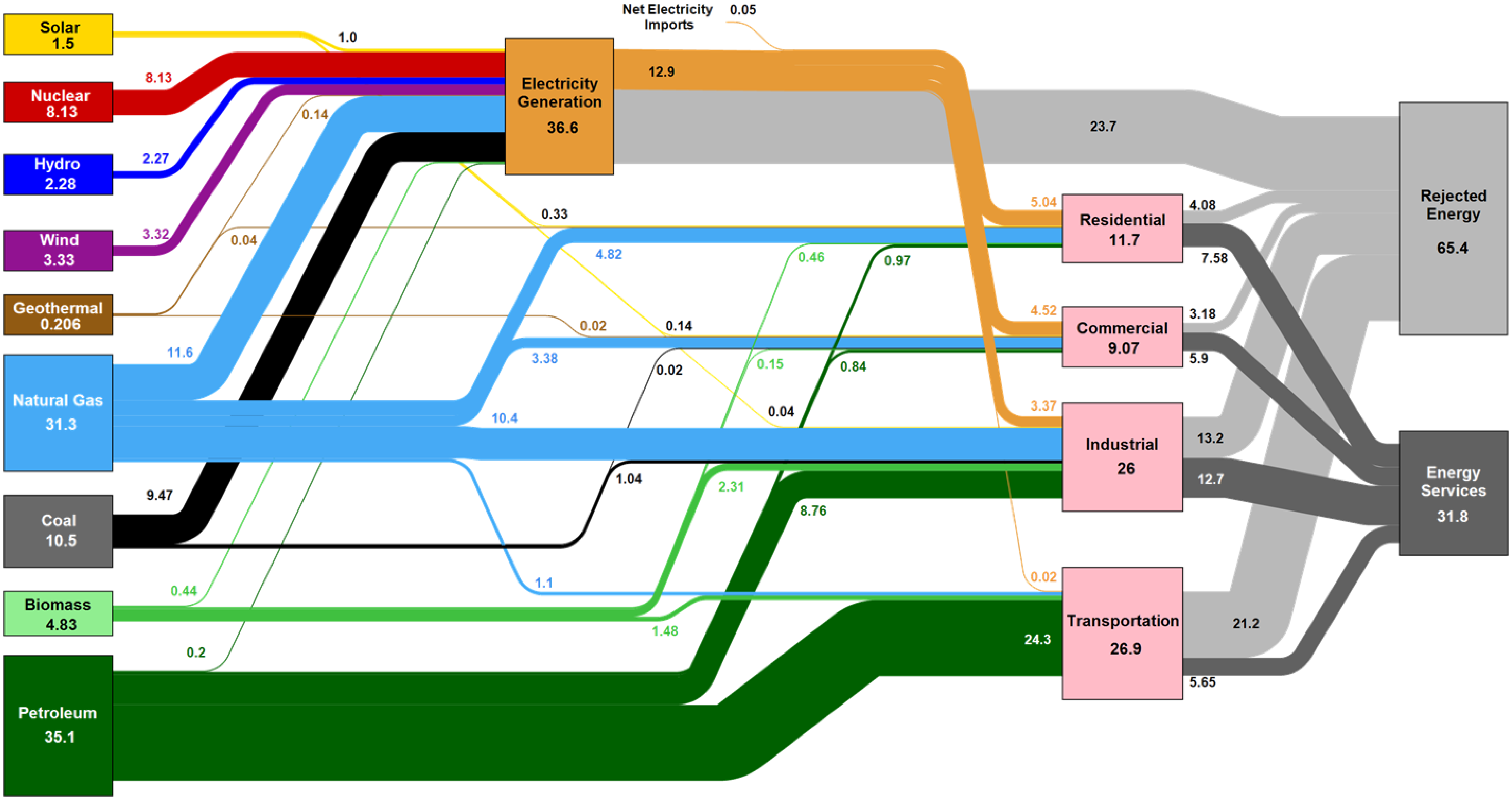
Oct 12, General Session, AM
New and Upcoming Features Andrew Lee, Dan Gunter

Posters
IDAES Diagnostics Toolbox Andrew Lee

IDAES Visualization and User Interfaces Dan Gunter



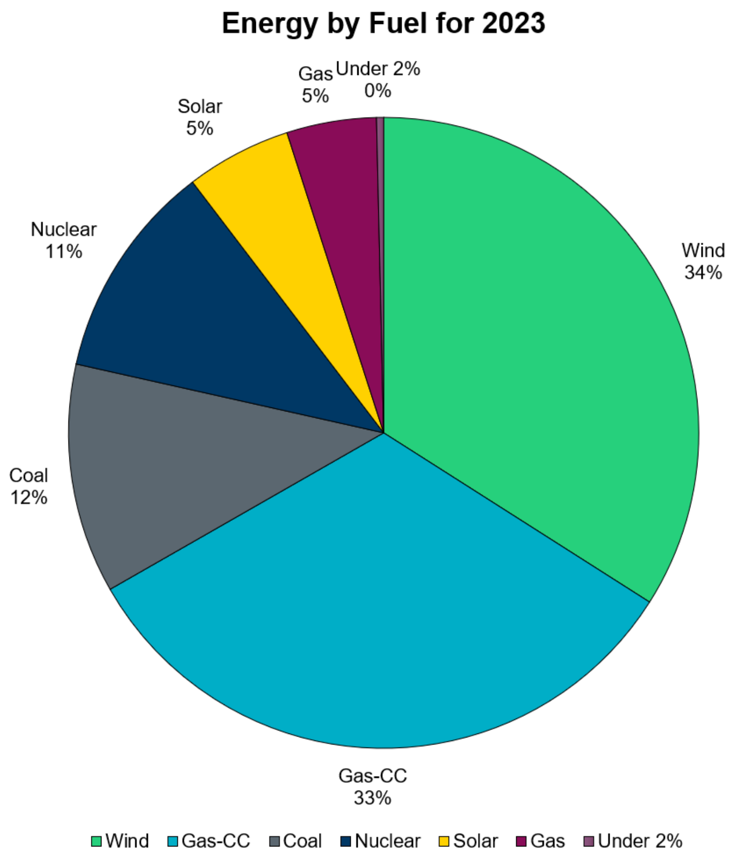
Estimated U.S. Energy Consumption in 2021: 97.3 Quads

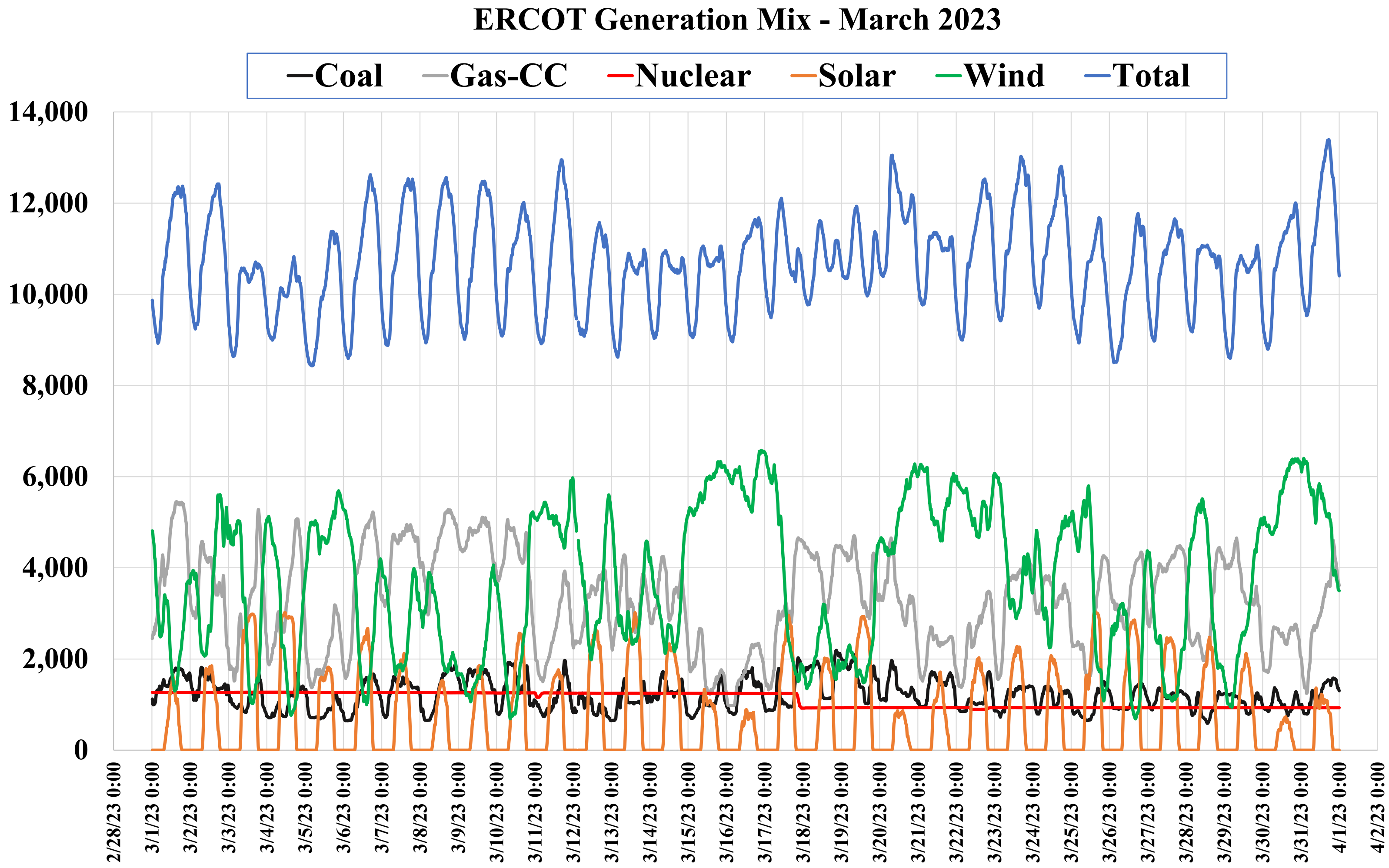


Source: LLNL March, 2022. Data is based on DOE/EIA MER (2021). If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports consumption of renewable resources (i.e., hydro, wind, geothermal and solar) for electricity in BTU-equivalent values by assuming a typical fossil fuel plant heat rate. The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 65% for the residential sector, 65% for the commercial sector, 21% for the transportation sector and 49% for the industrial sector, which was updated in 2017 to reflect DOE's analysis of manufacturing. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

Evolving Grid Increasingly Requires Flexibility

Data for Electric Reliability Council of Texas (ERCOT) ISO





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Source: https://www.ercot.com/gridinfo/generation

DOE's Office of Fossil Energy & Carbon Management (FECM) Strategic Directions and Priorities

- Advancing Justice, Labor, and Engagement
  - Justice
  - Labor
- Advancing Carbon Management Approaches toward Deep Decarbonization
  - **Point-Source Carbon Capture**
  - **Carbon Dioxide Conversion**
  - **Carbon Dioxide Removal**
  - Reliable Carbon Storage and Transport
- Advancing Technologies that Lead to Sustainable Energy Resources
  - **Hydrogen with Carbon Management (now funds Sim-based Engineering & IDAES-Core)**
  - **Domestic Critical Minerals Production**
  - Methane Mitigation

Next-generation multi-scale modeling & optimization framework

Fully Flexible	Model Libraries
Open Model Structure	Black Box Models
Optimization	Simulation
Dynamic	Steady-State
Conceptual Design	Case Studies
Academic	Commercial

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Transcending Boundaries

Built on

python

- High-level programming language
- Rich set of tools and libraries

PYOMO

- Open-source Python package
- Streamlined optimization modelling
- Development of numerical methods
- Interfaces with optimization solvers

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- Reusable and extensible unit models
- Equation-oriented approaches to physical property models
- Integrated with model identification and machine learning tools
- Advanced algorithms tailored to process design and optimization

IDAES is connecting cutting edge research with practice

- The IDAES team is developing a comprehensive, integrated set of PSE tools
  - Core unit modeling framework
  - Customized property packages
  - Initialization schemes
  - Diagnostics Toolbox
  - Custom system models
    - PC, NGSC, NGCC-based power generation, SOFC/SOEC, SMR, integrated power/hydrogen systems, hybrid energy systems, solvent-based carbon capture, direct air capture, etc.
  - Dynamic modeling
    - Dynamic unit model library
    - Model reduction techniques
    - Nonlinear state estimation and control
  - Data-driven modeling
    - ALAMO machine learning framework
    - Helmholtz energy equations of state fitting (HELMET)
    - General surrogate generation (PySMO)
  - Conceptual design
    - GDP-based superstructure design (Pyosyn)
  - Integrated process/market optimization
  - Process family design
  - Capacity expansion planning w/ reliability
    - Capacity expansion planning
    - Market modeling and simulation (Prescient)
  - Systems integration & materials design

IDAES provides both a vehicle for rapid dissemination of cutting-edge research results and an ecosystem for the maturation of those results into industrially-applicable capabilities.

IDAES Integrated Platform

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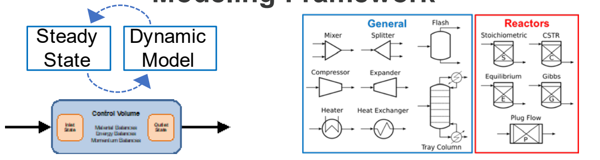
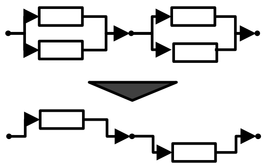
Modeling Framework



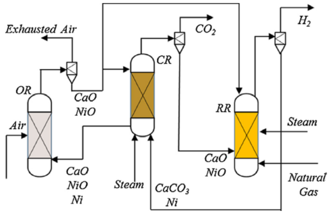
Hierarchical - Steady-State & Dynamic - Model Libraries

Conceptual Design

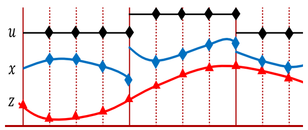


PYOMO GDP

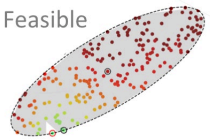
Plant Design Process Optimization



Process Operations Dynamics & Control



Uncertainty Quantification Robust Optimization

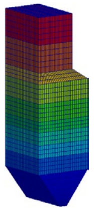


PyROS

AI/ML Surrogate Modeling

ALAMO

PySMO



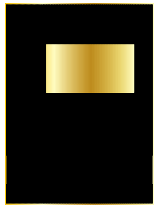
Enterprise Optimization Grid & Planning

Materials Optimization

MatOpt Nanomaterials optimization

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

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



NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Sandia National Laboratories | Carnegie Mellon | West Virginia University | UNIVERSITY OF NOTRE DAME | Georgia Tech

PYOMO

IDAES Institute for the Design of Advanced Energy Systems | python™

Gurobi	CPLEX	Xpress	CBC	Ipopt
GAMS	NEOS	Mosek	BARON	GLPK

Why IDAES?

- Hierarchical structure supports familiar modular assembly of flowsheets
- Integrated Ecosystem – all the tools you need in one place
  - dynamics, conceptual design, diagnostics, UQ, AI/ML, UI built
- Optimization focused – many commercial tools are designs for simulation
- Flexibility – object oriented programing allows more control over models
- Cost – open-source codebase, free of charge

Open-Source Platform

Website: https://idaes.org/

GitHub repo: https://github.com/IDAES/idaes-pse

Support: idaes-support@idaes.org

Ask questions, subscribe to our user and/or stakeholder email lists

Documentation: https://idaes-pse.readthedocs.io

Getting started, install, tutorials & examples

Overview Video

https://youtu.be/28qjcHb4JfQ

Tutorial 1: IDAES 101: Python and Pyomo Basics

https://youtu.be/_E1H4C-hy14

Tutorial 2: IDAES Flash Unit Model and Parameter Estimation (NRTL)

https://youtu.be/H698yy3yu6E

Tutorial 3: IDAES Flowsheet Simulation and Optimization; Visualization Demo

https://youtu.be/v9HyCiP0LHg

IDAES Contributions

Path 1: contribute to idaes-pse repository

Download idaes-pse repository → Model Development → Open GitHub PR → Merge Code

- **Download idaes-pse repository**: Get idaes. Follow standards and examples
- **Model Development**: Local system. Build and test models
- **Open GitHub PR**: Contribute models, tests, and examples to IDAES
- **Merge Code**: Rigorous testing and structural analysis

Path 2: create GitHub repository and make idaes-pse a dependency

IDAES Projects Span Multiple Time-Scales

- Technoeconomic and market analysis of SOEC/SOFC-based hydrogen and electricity co-production systems (hours → years)

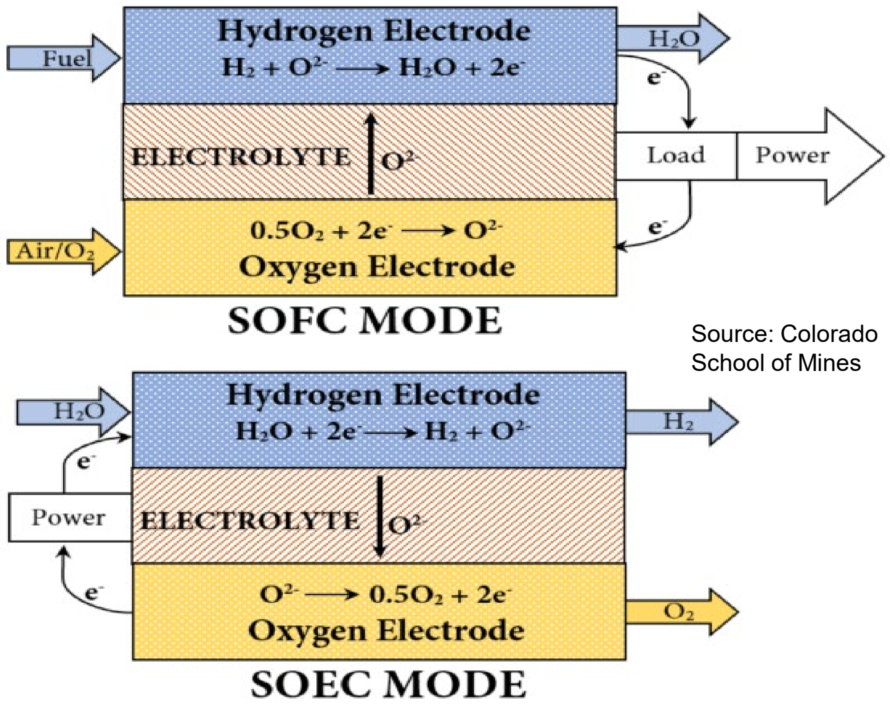
- Dynamic & health modeling, control, and optimization of SOEC/SOFC-based systems (seconds (dynamic operation) → years (health))

- Integrating short-term operational realities (e.g., unit commitment and dispatch) into long-term expansion planning models (minutes → decades)

Solid Oxide Cell (SOC)-based Integrated Energy Systems (IES)

<u>Key Challenge</u>

- How can we **best operate and control** SOC-based IES for **mode-switching (H_2/power)**, while **minimizing degradation** over long-term flexible operation?
    - SOCs operate at much **higher temperatures** than other fuel cell/ electrolysis technologies
    - While high-temperature operation offers **higher current density** and **efficiency**, it also poses significant challenges:
        - Additional **heat exchange** equipment
        - Accelerated **degradation**
        - **Tight controls** for optimizing performance and health during setpoint transitions and mode-switching operation



Source: Colorado School of Mines

Operating principles for H_2 fuel in SOFC mode and steam electrolysis in SOEC mode.

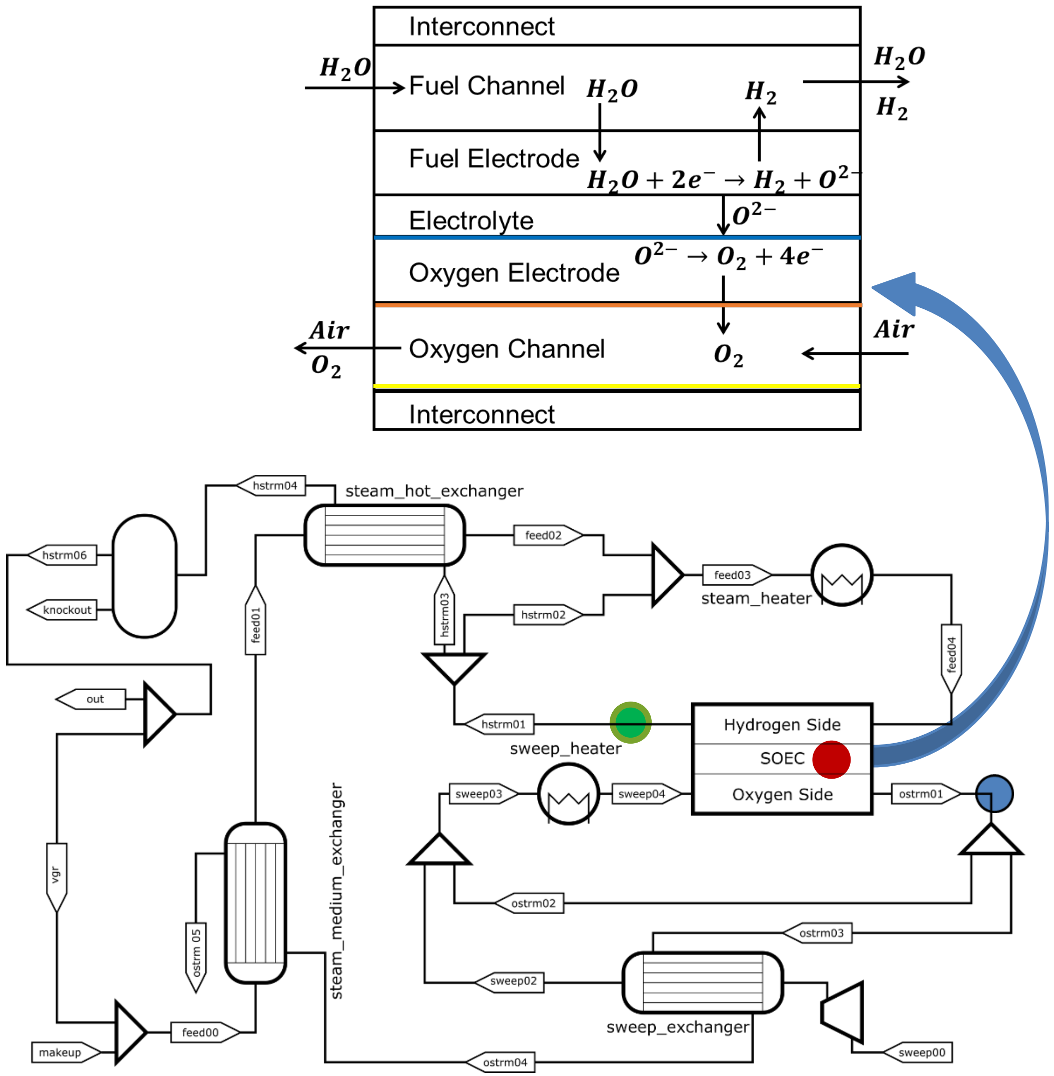
Optimization of SOC-based IES Flexible Operations
Dynamics, Control, and Health Modeling

<u>Technical Approach</u>

- **Dynamic Modeling**
  - Develop **first-principles dynamic model** of SOC-based IES using **IDAES** software
- **Process Control**
  - Develop **classical and advanced process controls** for effective thermal management and mode-switching operation
- **Health/Degradation Modeling**
  - Develop first-principles sub-models for **physical and chemical degradation**, as well as their **synergistic effects**, to quantify impact on cell health
- **Optimization**
  - Optimize **performance** and **health** of SOC-based IES for **long-term flexible operation**

Dynamic Model of H_2-fueled SOC-based IES for Mode-Switching

- **IDAES** open-source, equation-oriented modeling and optimization framework (Lee et al., 2021)
- **SOC dynamic model** (Bhattacharyya et al., 2007)
  - First-principles, non-isothermal, planar
  - 1D channel; 2D electrodes, electrolyte, and interconnect
  - H_2 fueled in power mode
- Equipment models for **thermal management**
  - 1D multipass crossflow recuperative heat exchangers
  - 1D crossflow trim heaters
- System **performance constraints**
  - Maximum H_2O outlet concentration to ensure good conversion
  - Minimum O_2 in sweep outlet to prevent oxidation
  - Max cell thermal gradient to avoid degradation



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).

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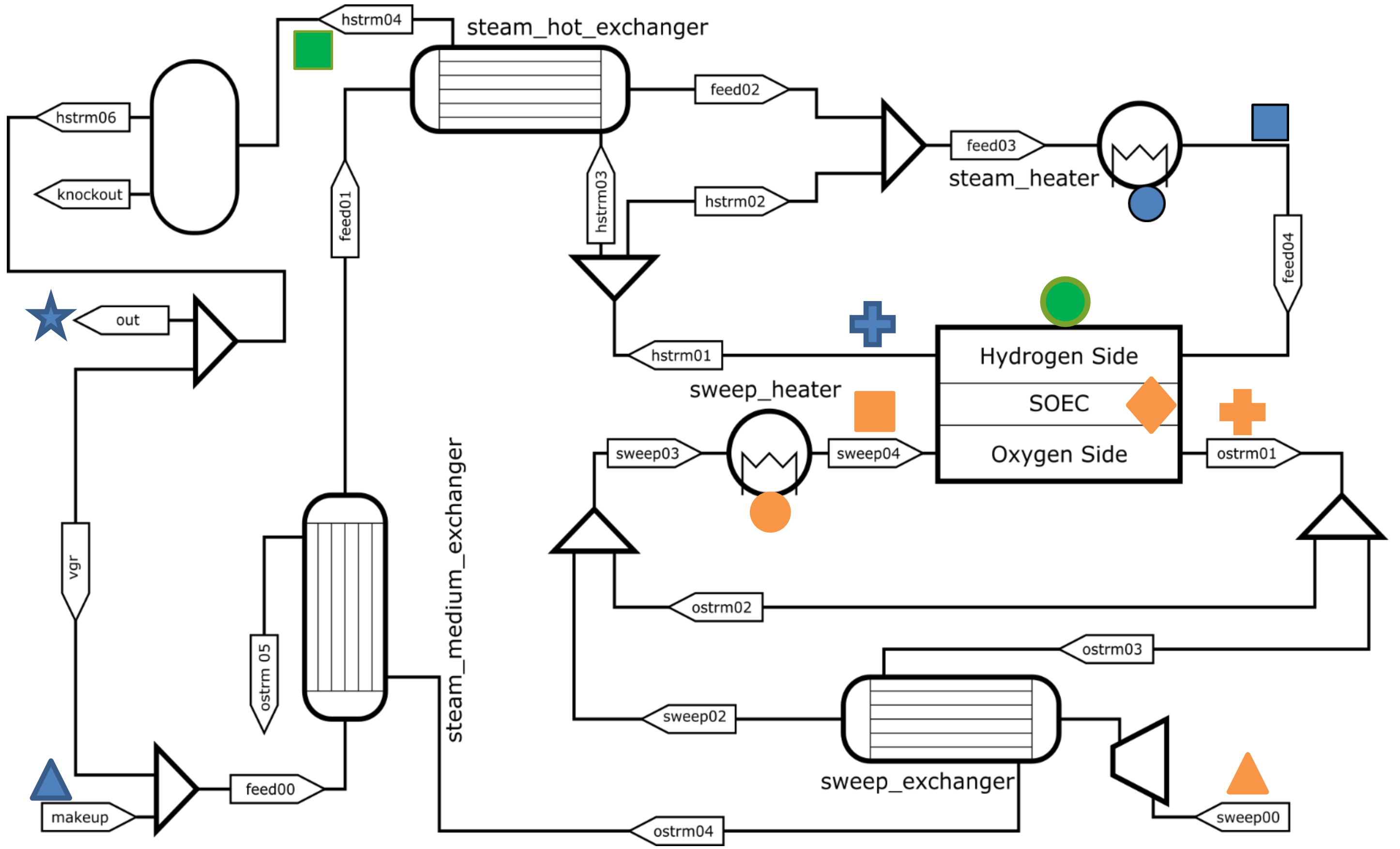
Process Control for SOC-based IES Mode-Switching Operation

- **Classical Control: Proportional-Integral-Derivative (PID)**
- **Nonlinear Model Predictive Control (NMPC)**



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*

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

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NMPC for SOC-based IES Mode-Switching Operation

- NMPC is well suited to **highly interactive manipulated variables** and **constraint handling**
- NMPC **objective function**

$$f_{\text{obj}} = \sum_{i=0}^{N} \rho_{\text{H}_2} \left(y_i - y_i^R\right)^2 + \sum_{i=0}^{N}\sum_{j\in J} \rho_j \left(u_{ij} - u_{ij}^R\right)^2 + \sum_{i=0}^{N}\sum_{k\in K} \rho_k' \left(x_{ik} - x_{ik}^R\right)^2 + \sum_{i=1}^{N} \rho' \left(\nu_i - \nu_{i-1}\right)^2 + \rho_s \sum_{i=0}^{N}\sum_{z=1}^{z_L} \left(p_{iz} + n_{iz}\right)$$

Trajectory tracking of H_2/power production rate

Deviations of manipulated variables (u_{ij}) and controlled variables (x_{ik}) from reference values

Rate of change penalties on trim heater duties

ℓ_1-penalties for temperature gradient constraints

- To prevent thermal degradation over time, the temperature gradient along the cell length (z-direction) is constrained to be below dT/dz_{ub} K/m
- An ℓ_1-penalty relaxation treats them as soft constraints with non-negative slack variables p and n penalized in the objective

$$dT/dz - dT/dz_{ub} \leq p \quad \textit{and} \quad - dT/dz - dT/dz_{ub} \leq n$$

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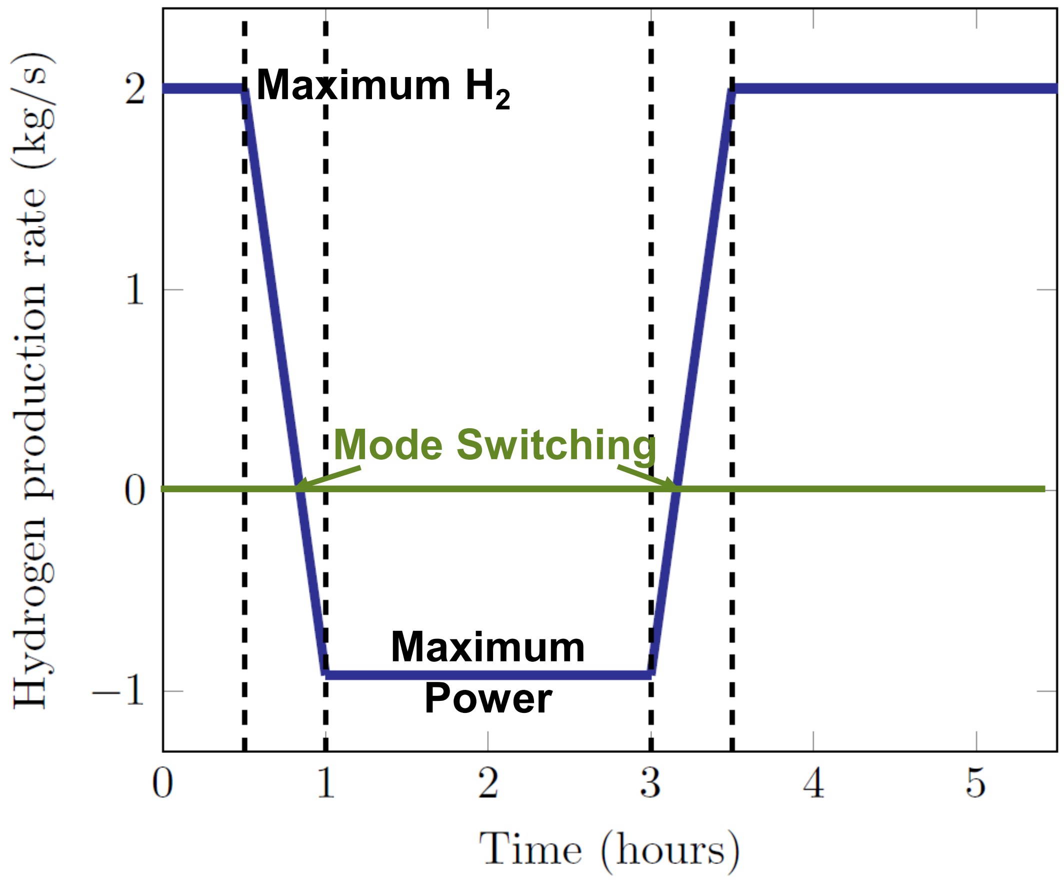
SOC-based IES Mode-Switching Operation

- **Mode-Switching**
  - Maximum H_2 (2.0 kg/s) to maximum power (-0.92 kg/s) and back to maximum H_2
  - Ramps performed over 30 min, followed by 2 hours of settling time
- **IDAES Solution Approaches**
  - Classical control: PETSc variable-step implicit Euler dynamic integrator
  - NMPC: **Full-discretization** NLP with IPOPT optimizer



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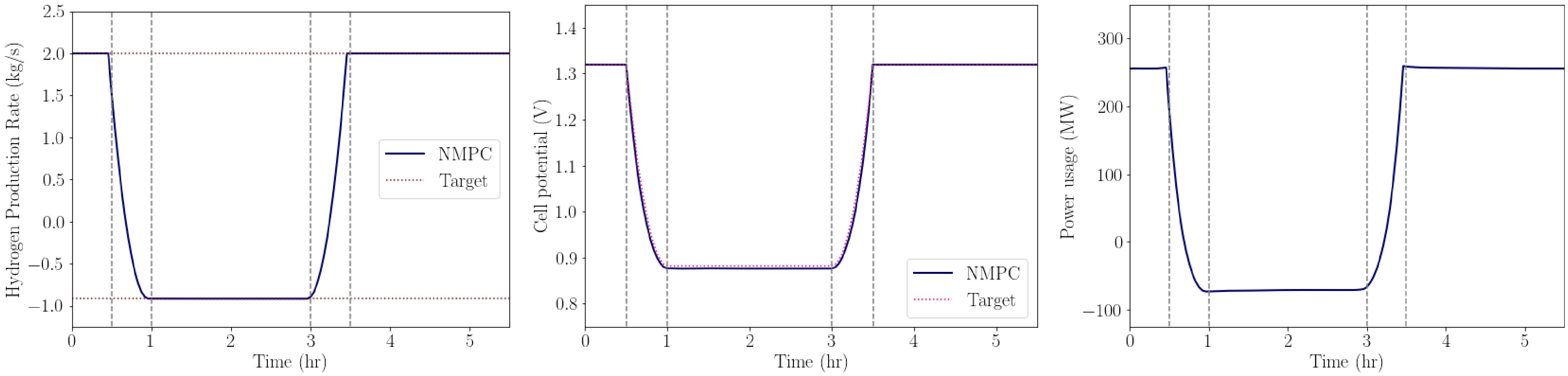
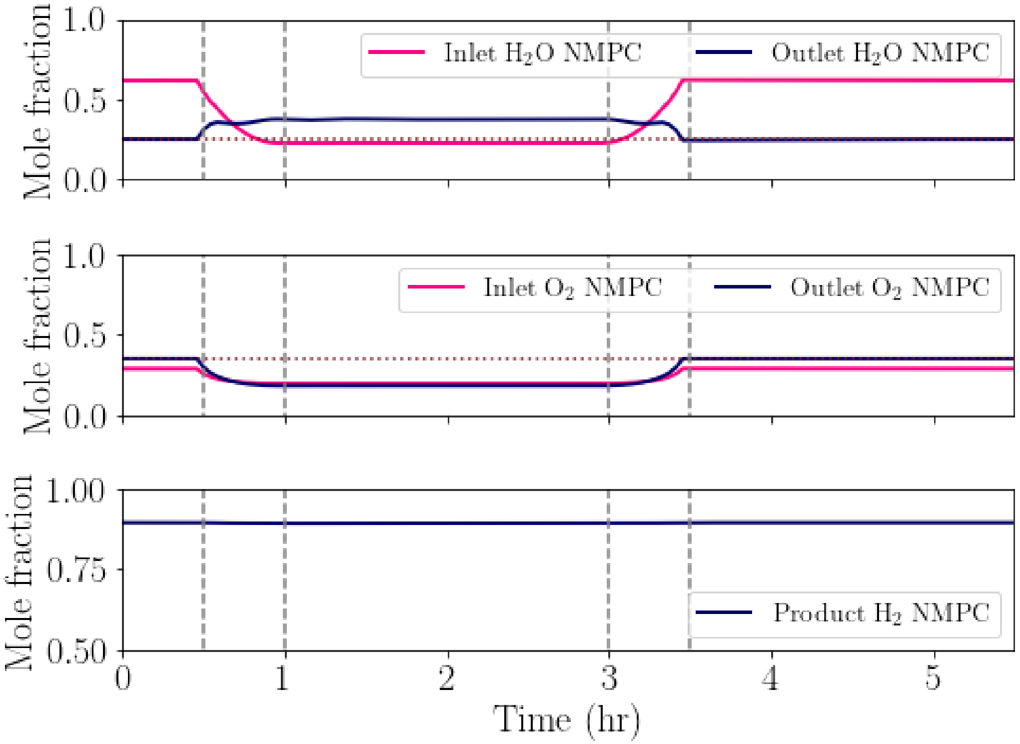
NMPC Results for SOC-based IES Mode-Switching Operation

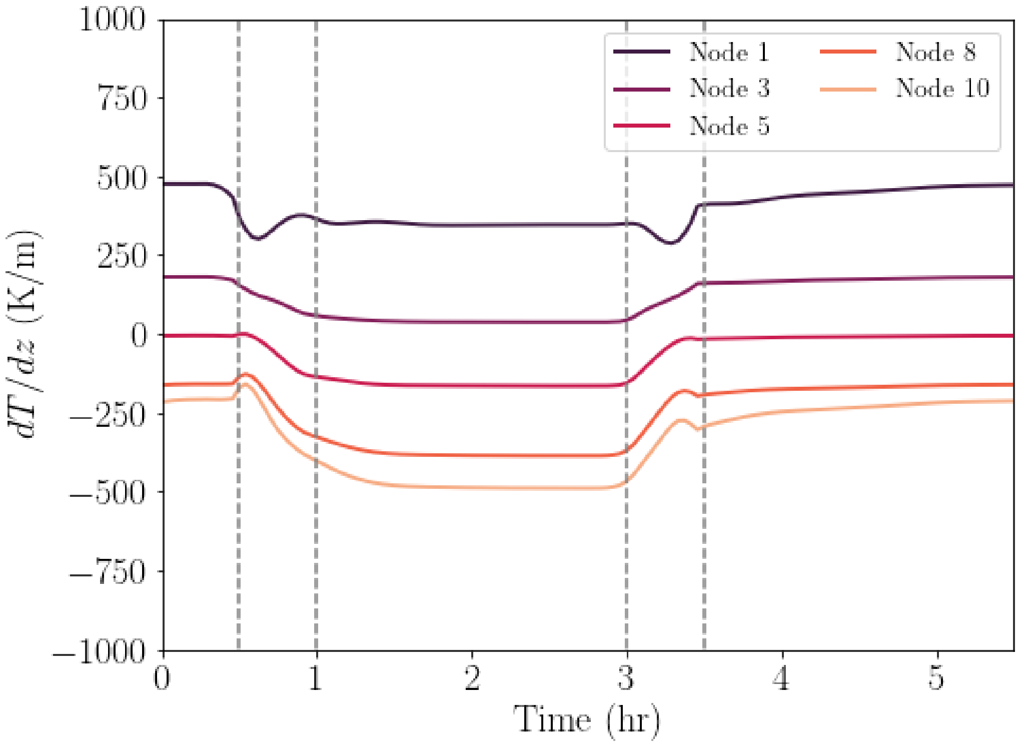


Hydrogen production tracking has no overshoot, and is correlated to **cell voltage** and **total power usage**

NMPC Results for SOC-based IES Mode-Switching Operation

- **Performance constraints are satisfied**
  - Maximum H_2O in outlet to ensure good conversion in SOEC mode
  - O_2 in sweep outlet ≤ 35% (mole basis) to prevent oxidation
  - Conversion of steam to H_2 ≥ 75% to avoid steam starvation
  - Maximum cell thermal gradient ≤ 1000 K/m to avoid stress





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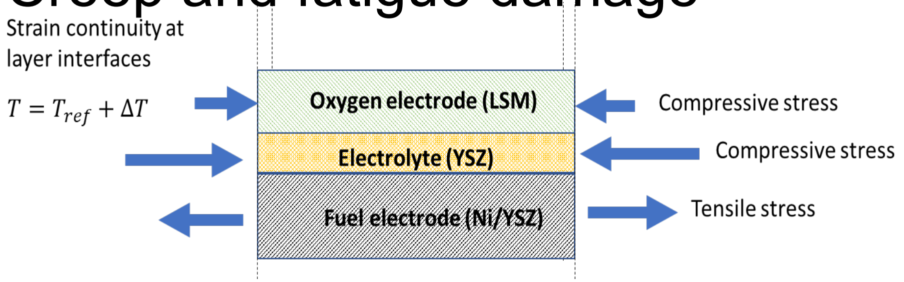
SOC Health/Degradation Modeling

- **Physical Degradation**
  - High spatial and temporal temperature gradients
  - Thermo-mechanical stresses
  - Creep and fatigue damage



- **Chemical Degradation (H_2 fuel)**
  - Oxygen electrode
    - Chromium oxide scale growth
      - Increased local **ohmic resistances**
    - Lanthanum zirconate scale growth
    - LSM-YSZ coarsening
  - Fuel electrode
    - Ni agglomeration and volatilization
  - Electrolyte
    - YSZ electrolyte delamination

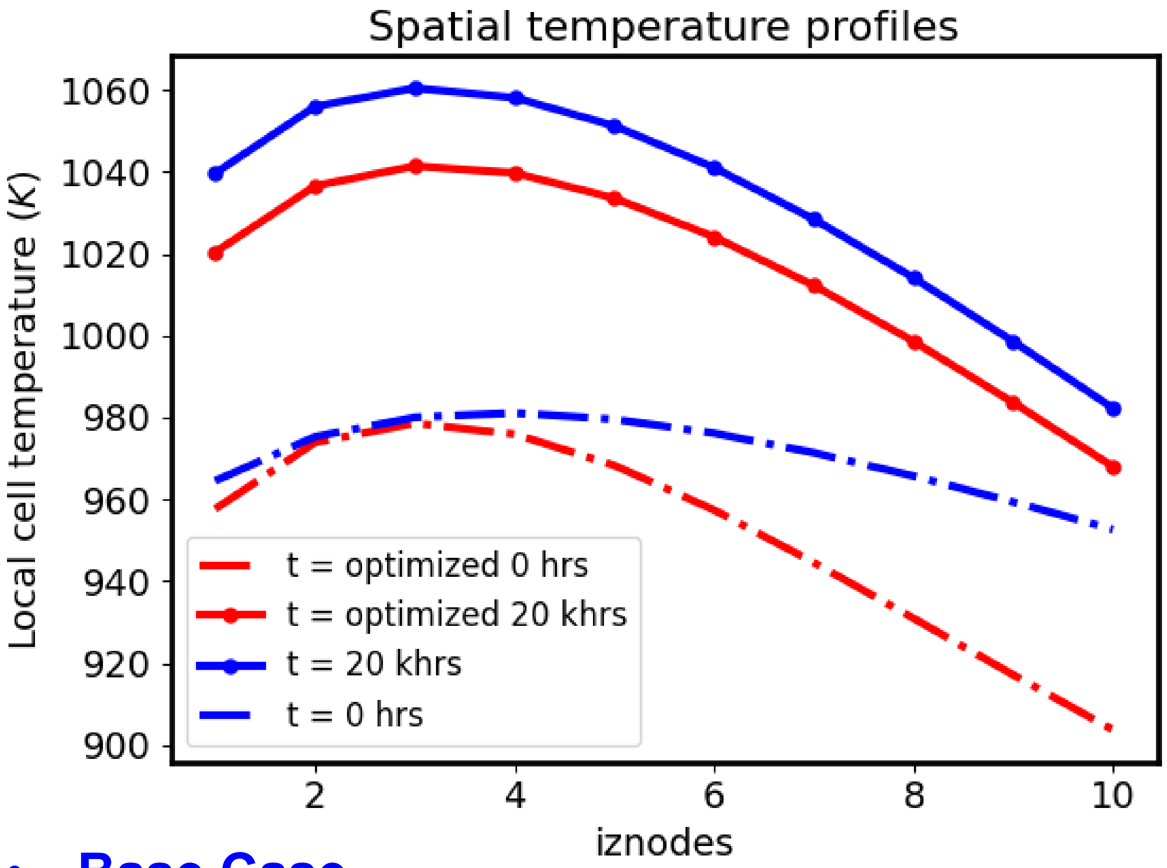
- **Synergistic Effects**
  - Chemical degradation negatively impacts physical degradation by:
    - increasing local **Ohmic resistance** and cell temperature
    - affecting **thermo-physical properties** of the ceramic materials, which result in variation in the cell thermal profile
    - affecting **mechanical properties** of cell components such as Young's modulus and Poisson's ratio

Case Study: SOEC Health Optimization over Long-Term Operation

- **20,000 hrs** of operation
- **Electrolysis mode**
  - High H_2 production rate: 1.5 kg/s
- Chemical degradation (O_2 electrode)
- **Health Optimization Case**
  - Minimize final ohmic resistance

$$\min R_{ohmic,tf}$$

  - Decision variables at every time point
    - Fuel and oxygen trim heater duties
    - Fuel and oxygen inlet flowrate
    - Fuel and oxygen recycle ratio
  - Quasi-steady optimization
    - Dynamic degradation model
    - Steady-state SOEC system model



- **Base Case**
  - No optimization for health/degradation
  - Constant inlet temperatures over operating horizon from steady-state optimization at t=0 hrs to maximize efficiency

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Case Study: SOEC Health Optimization over Long-Term Operation

High H_2 production rate : 1.5 kg/s					
Objective Function	$\left.\frac{dT}{dz}\right\|_{max}$ (K/m)	T_{core} (K)	$\eta_{average}$	R_{ohmic} (mΩ/ khr)	$P_{specific}$ (MWh/kg H_2)
Base Case	1020	1033	**0.872**	0.34	**38.05**
Degradation Optimization Case: Minimize final resistance	**980**	**1020**	**0.875**	**0.26**	**38.15**

- About **25% reduction in resistance** growth rates (R_{ohmic})
- System **efficiency** ($\eta_{average}$) and **power requirement** ($P_{specific}$) remain **unchanged**
  - **Resistive heating in trim heaters instead of inside the cell**
- Minimizing resistance can keep absolute cell temperatures (T_{core}) in control
- Thermal gradients constraints ($\left.\frac{dT}{dz}\right|_{max}$ < 1000 K/m) **remain feasible** after 20,000 hrs of optimized performance

Please stop by poster for more details/results on SOC health modeling and optimization.

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Summary

- **IDAES** offers an open-source modeling framework for **optimization** of the operation, control, and health of **flexible SOC-based IES.**
- **NMPC** provides **accurate H_2/power production setpoint tracking** during mode-switching operation.
- Results for **SOEC health optimization** over **long-term operation** show that:
  - ohmic resistance growth and cell temperature are reduced,
  - H_2 production rate and efficiency are maintained, and
  - thermal gradients are kept under control.

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Future Work

- Enhance **NMPC** to maximize SOC system performance for **"faster" mode-switching** operation, while **reducing temperature gradients** to benefit cell health
- Analyze **synergistic effects** of **physical and chemical degradation** for mode-switching operation
- **Optimize SOC system performance** over **operational lifetime** using measure of **health** on **economics**
- Develop prototype of **multiple timescale computational approach** in IDAES for solving coupled dynamic simulations of long-term flexible operation and degradation

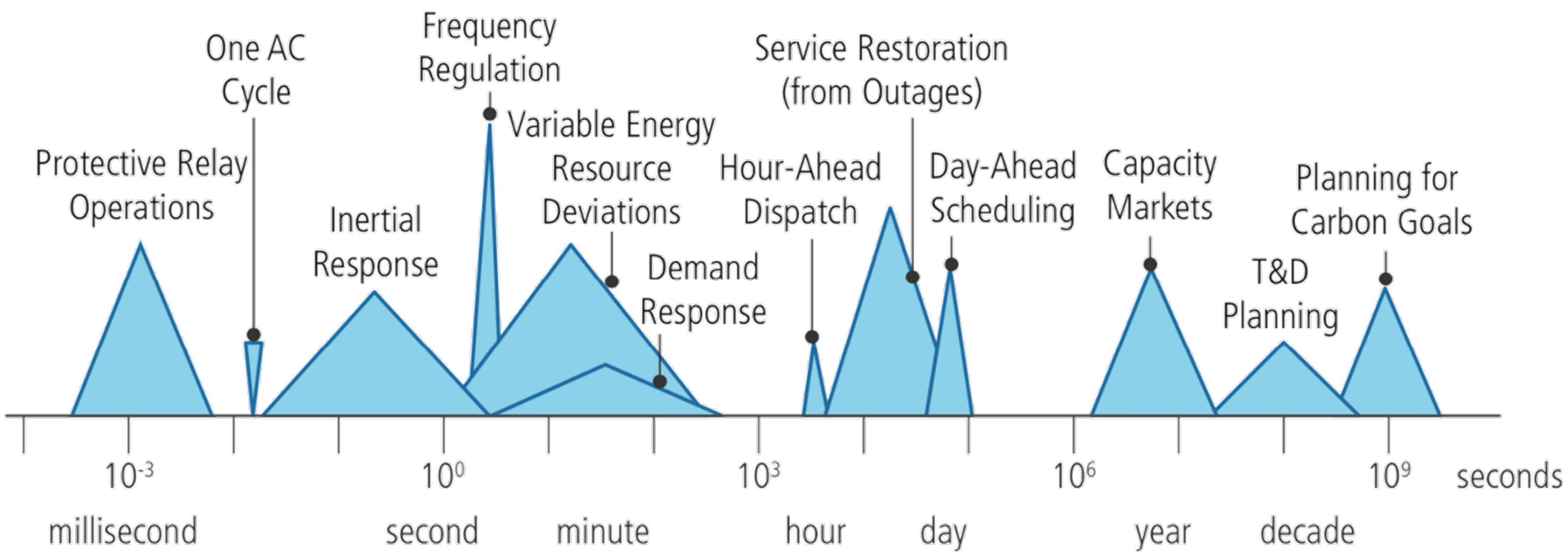
IDAES Projects Span Multiple Time-Scales

- Technoeconomic and market analysis of SOEC/SOFC-based hydrogen and electricity co-production systems (hours → years)

- Dynamic & health modeling, control, and optimization of SOEC/SOFC-based systems (seconds (dynamic operation) → years (health))

- Integrating short-term operational realities (e.g., unit commitment and dispatch) into long-term expansion planning models (minutes → decades)

Expansion Planning Modeling: Will Technology be Deployed?



Real-Time Operations	Electricity Grid Dispatch, Power Flow	Capacity Expansion 20-30 Year Horizon	Energy Economy Models
High frequency dynamics	Complex effects of new generators	Difficult to value flexibility, reliability	Long time horizons Macro-economics

Process/Generator – Integrated Energy Systems

Design, Operation/Control, Dynamics, Multiple Products

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Expansion Planning Problems Are “Huge”

- At the core, an expansion planning model considers
  - Systems with **>$\mathbf{10^2}$** generators, **>$\mathbf{10^3}$** transmission lines,
  - Balancing loads over each of **$\mathbf{10^6}$ time periods**,
  - With numerous opportunities to install, extend, and retire assets,
  - And significant uncertainty in all parameters (generator costs, available technology, load growth and patterns, renewable resources),

- Too large to “directly solve”

- Numerous simplifications and approximations to develop “tractable” models
  - ACOFP → DCOPF → Transshipment
  - Full network → “skeletonized” network → “copper plate”
  - Individual generators → generator clusters
  - Full time horizon → representative days → representative loads
  - Discrete decisions → continuous relaxations

- Simplifications for tractability will impact accuracy

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Why is IDAES Developing Expansion Planning Models?

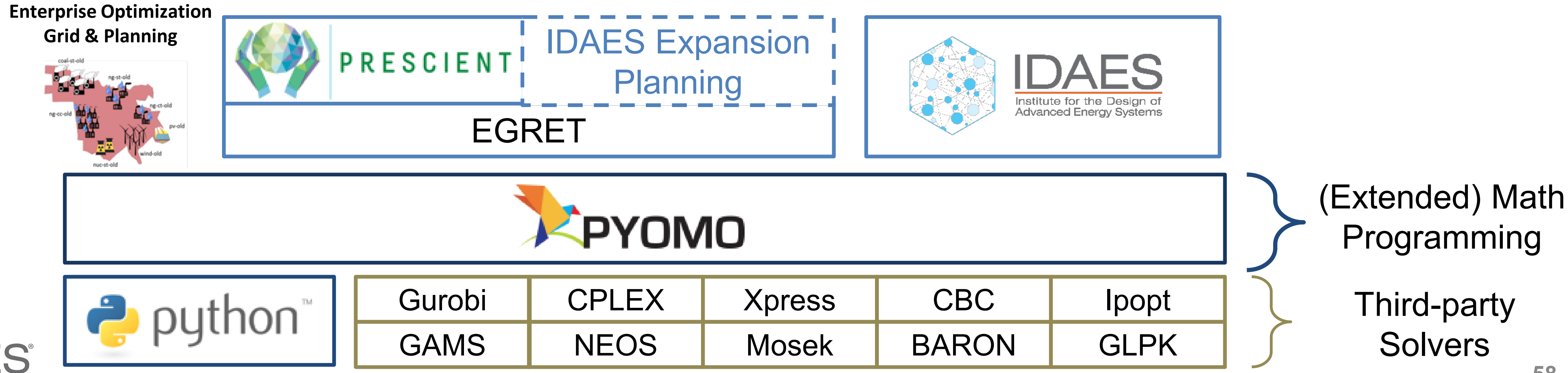
- Integrated Energy Systems must be designed for the *system*
  - Designing in isolation (e.g., “max efficiency”) does not guarantee participation / revenue from the market

- Existing expansion planning models focus primarily on *capacity*
  - Operability (e.g., the role of **dynamics, flexibility, and uncertainty**) is not explicitly included, leading to results that overvalue LCOE and undervalue dispatchability and flexibility

- Extending expansion planning models is more than just adding features
  - Scaling up the model requires exploring new algorithmic approaches to solving the model. **Model is open, allowing for customization for the problem you are interested in addressing**

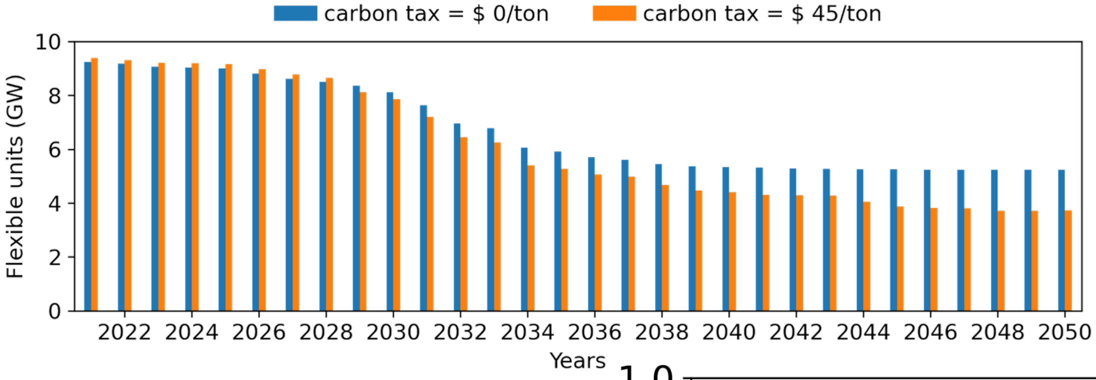
Current IDAES Expansion Planning Activities

- Develop reliability models and algorithms (Carnegie Mellon University, Seolhee Cho and Ignacio E. Grossmann)
  - Improve valuation of **flexibility**
  - Incorporate **resilience with reliability**
  - Expand to new case studies (partnering with California Energy Commission)
- Model maturation (Sandia National Laboratory)
  - **Generalizing / standardizing the models**, leveraging standardizing modeling components from **EGRET**
  - **Generalizing / standardizing algorithms** (remove explicit ties to case studies)

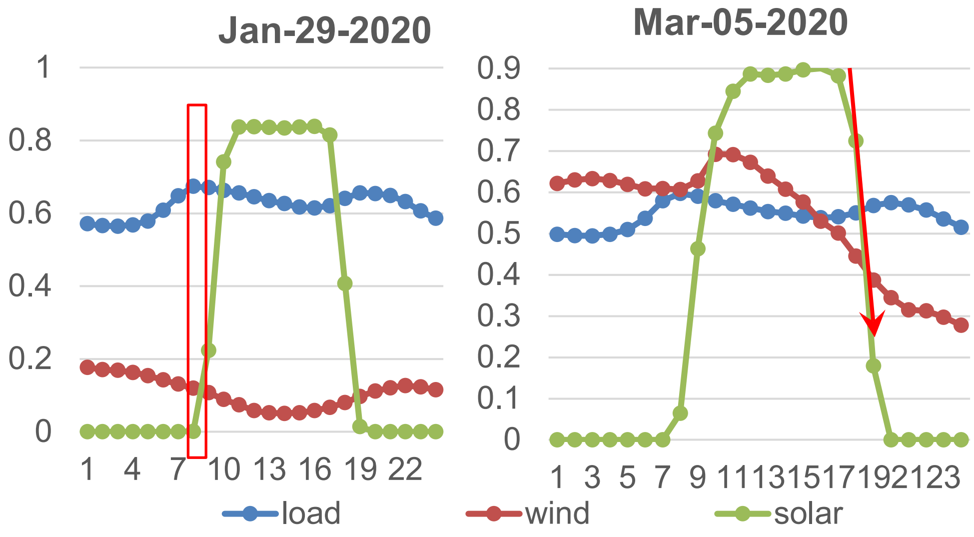


Quantifying the Impact of Flexibility

- Expansion planning with SPP case study **(hourly load balance with seasonal representational days)**
  - Results indicated significant reduction of installed flexible generation **with higher carbon tax**
    - Gas turbine, internal combustion turbine units
    - Lower efficiency, higher relative emissions
  - ***Counter-intuitive result***



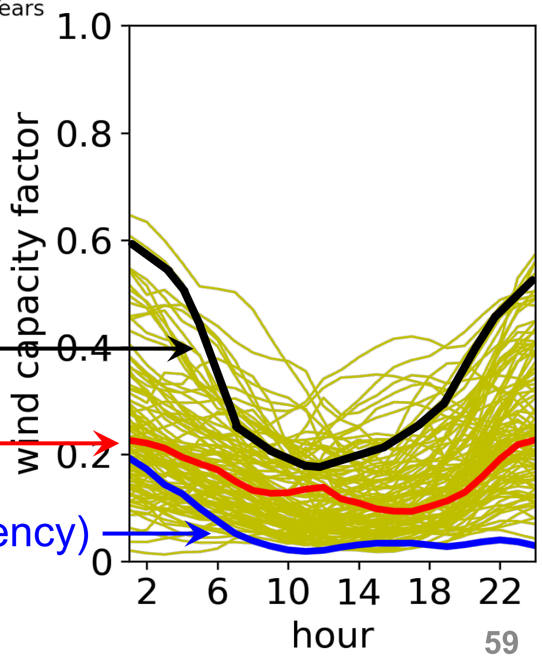
- Root cause: "representative" days did not capture
  - High ramp rates (volatility)
  - Low non-dispatchable generation (intermittency)



Scenario with high ramp rates (volatility)

Representative day

Scenario with low generation levels (intermittency)



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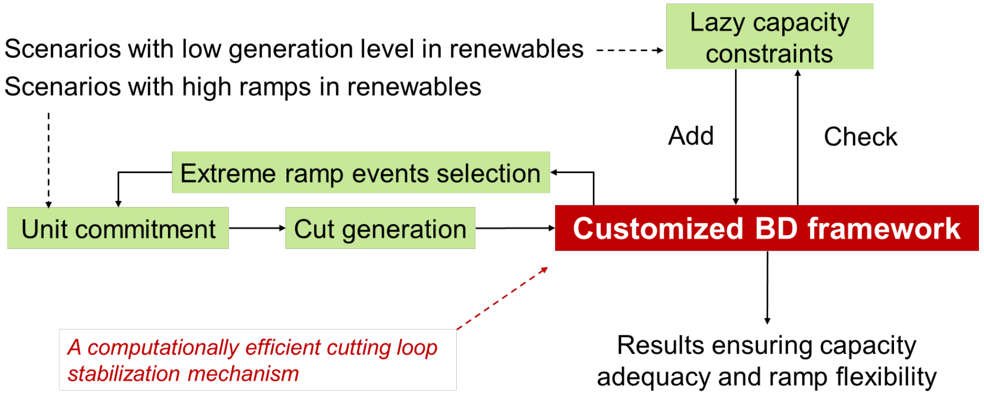
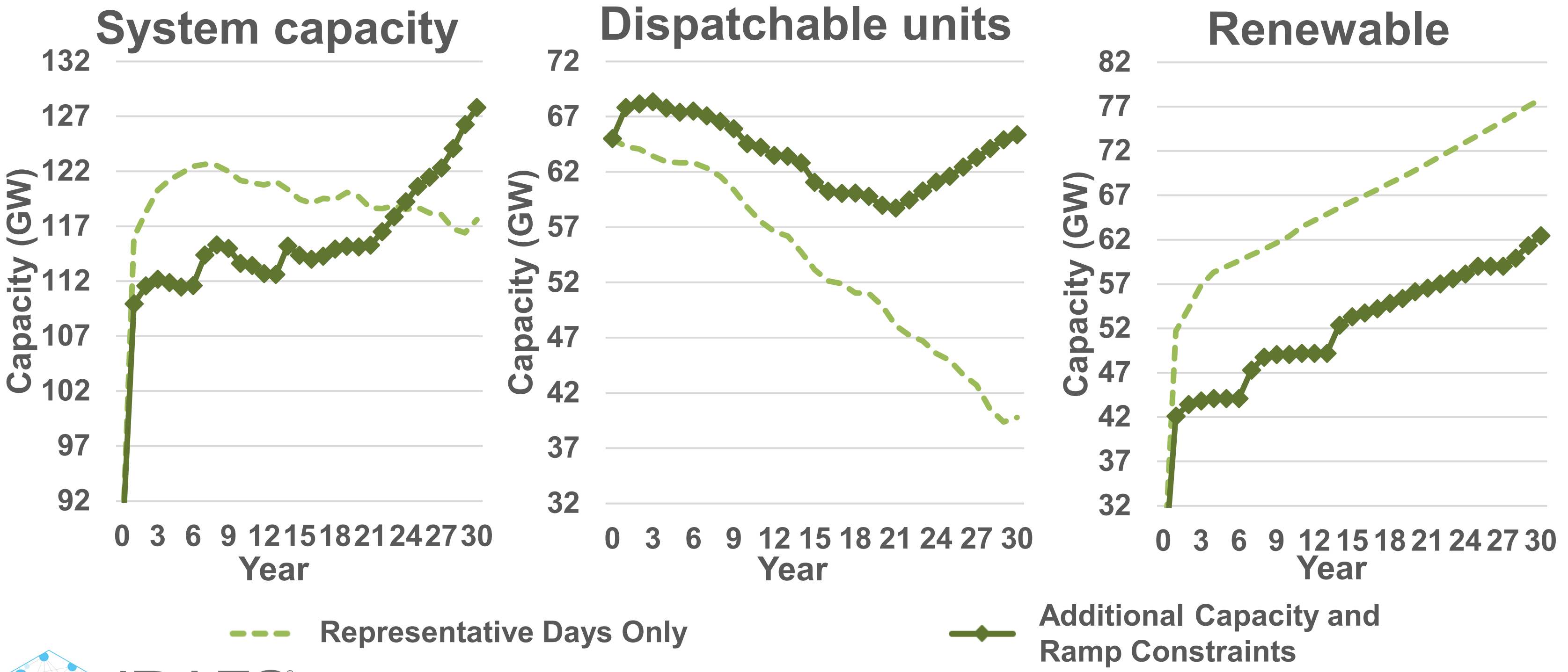
Accounting for Intermittency and Volatility

- "Non-representative" capacity and ramp scenarios critical in understanding dispatchable unit requirements
- Modified algorithm provides insights into low renewable capacity and/or rapid dispatchable ramp scenarios
  - Lazy capacity constraints
  - Extreme ramp events





- "Representative Days Only" underestimates total required capacity
- More dispatchable capacity required with additional capacity constraints and ramp events

* SPP scenarios under high carbon tax

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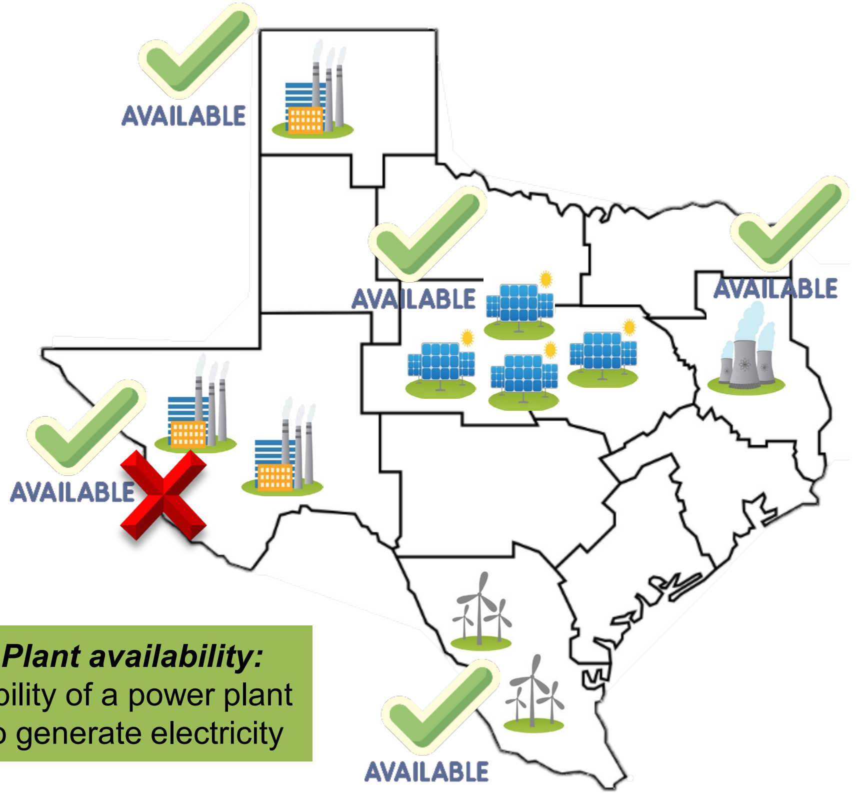
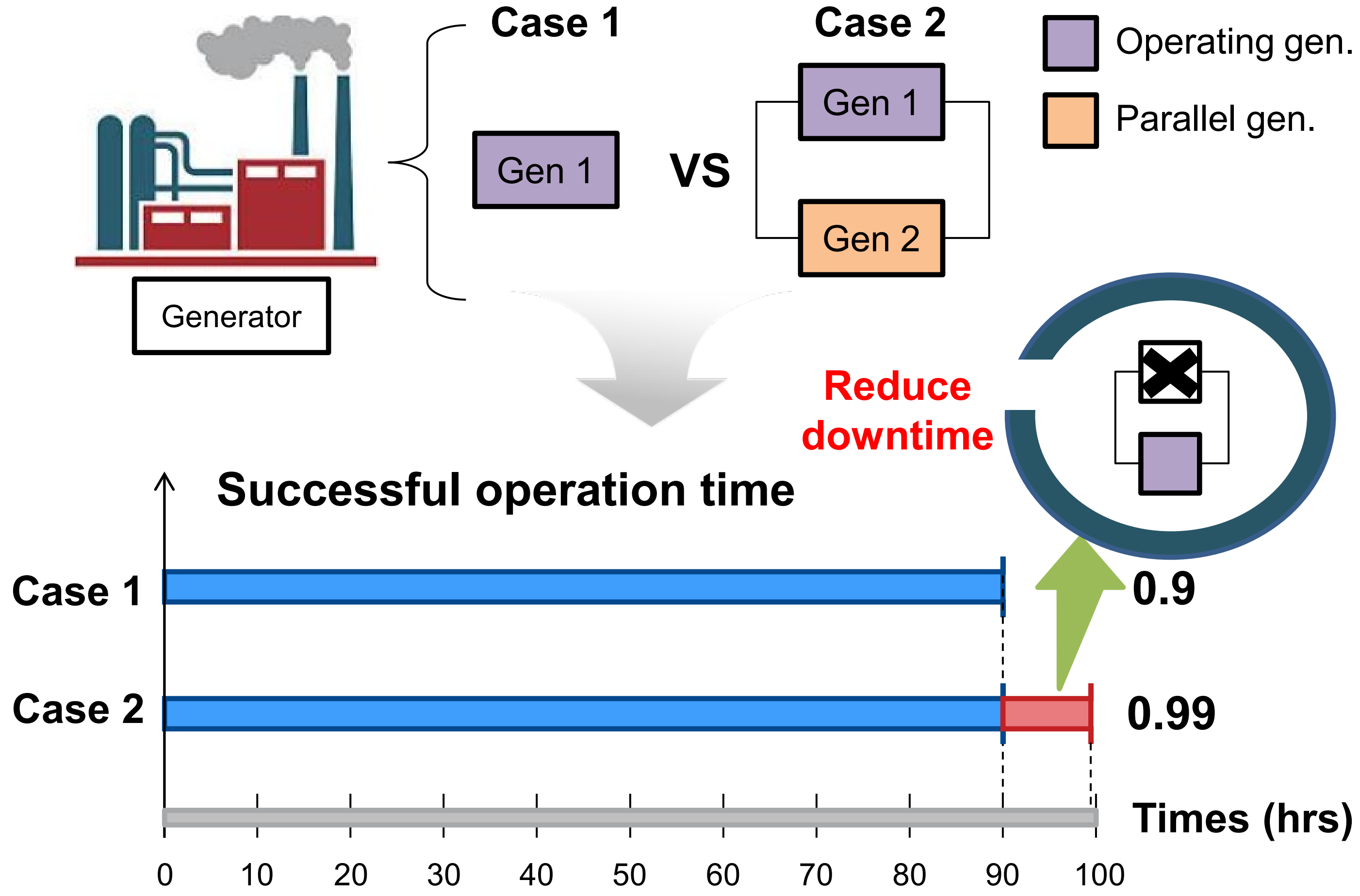
How to Improve Reliability - Redundancy

- Power systems reliability can be enhanced by improving availability of power plants.
- *Redundancy* Adding units in parallel enables a power plant to be highly available.



Plant availability:
Ability of a power plant to generate electricity

Power **plant availability** ↑ ↓
→ Power **systems reliability** ↑ ↓

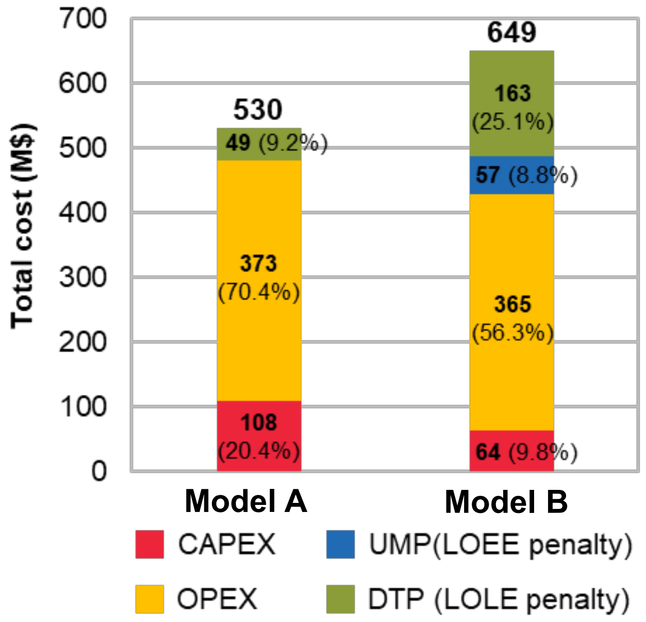


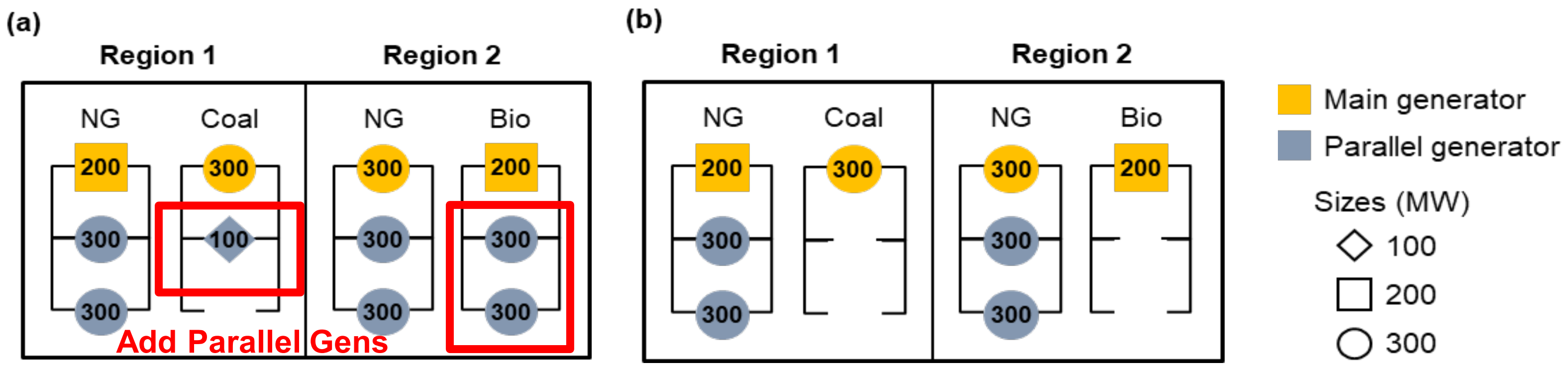
Including The Cost of Not Meeting Demand – Optimizing Considering Reliability

Illustrative example (2 regions, 3 types of power plants (Coal, natural gas (NG), and biomass (Bio))

Cost results

(a) Model A (w/ reliability), **(b)** Model B (w/o reliability)





(a) Model A (w/ reliability), **(b)** Model B (w/o reliability)

- Model A requires **higher CAPEX and OPEX** due to having **more parallel generators**.
- However, **lower reliability penalties are occurred in Model A** as the model considers slack capacity to reallocate the load demand when the generators fail.
- Model B has **lower CAPEX and OPEX** than Model A but incurs in **higher reliability penalties** due to its insufficient capacity.
- The more reliable design obtained by Model A enables the power generation systems to have a better economic performance than Model B.

LOLE (Loss Of Load Expectation) - time of not satisfying the load demand

LOEE (Loss of Energy Expectation) - The amount of demand that the system cannot satisfy

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CEC Case Study: Planning of Reliable Power Generation Systems with High Renewable Penetration

Case study with new capability (results expected 3/31/2024)

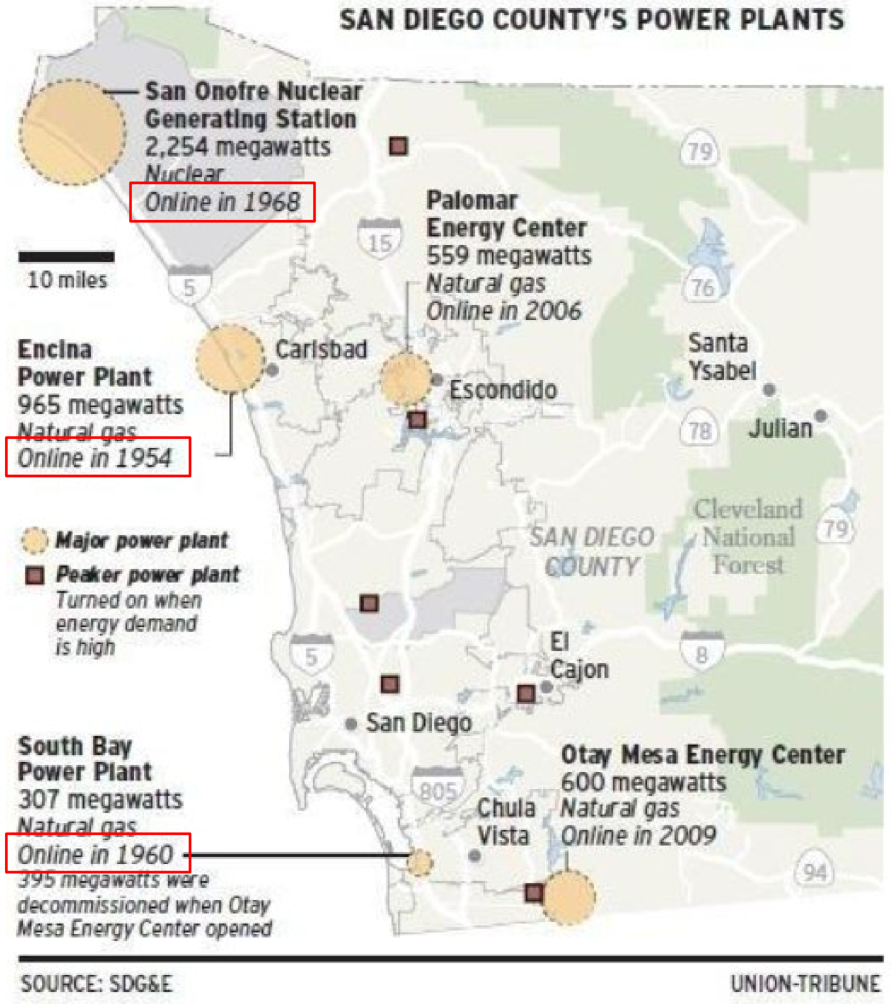
- Target area: San Diego County, California

Problem description

- For 5 major existing conventional power plants and peakers (supplementary power plants) ,
  → **determine the time to retire/decommission**
  (Installation of new conventional plants and peakers is prohibited)
- For renewable generations such as wind turbines and PV panels,
  → **time, size, location to newly install**
- By installing *batteries*, power systems reliability can be further improved.
  → **determine the time, size, location to newly install/retire, and operational strategies**
- Alternate cost of decarbonization with conventional plants with capture.

***Practical constraints**

- Target renewable generation share, CO_2 emission limit, LOLE < 0.1*



[Simplified power plants map of San Diego County]

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[1] California Peaker Power Plants: Energy Storage Replacement Opportunities, PSE Healthy Energy, 2020

*: 1 day outage with an event in 10 years

Summary

- **IDAES is a multi-lab initiative created to support long term DOE goals**
  - Decarbonizing power by 2035, economy by 2050
  - Evolving energy ecosystem requires greater flexibility & integration
- IDAES enables unique and innovative analyses across multiple time-scales
- Significant capabilities have been built to examine the market potential and controllability SOFC/SOEC-based integrated power and hydrogen systems
- Upcoming analysis entails better integrating operational realities into long term expansion planning of reliable, decarbonized electricity grids, with a key case study in collaboration with CEC.

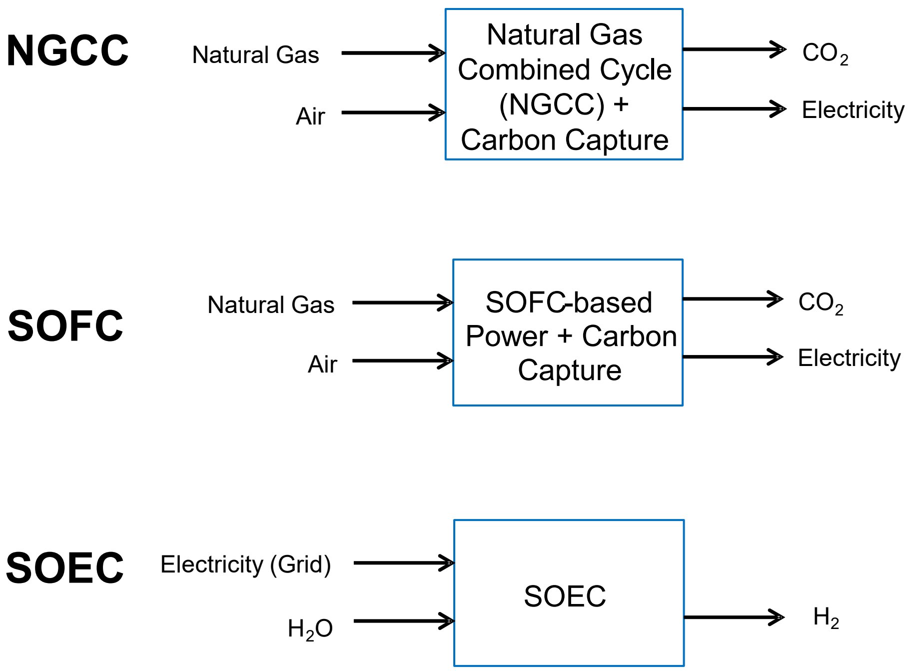
Useful Costing References for IES Work

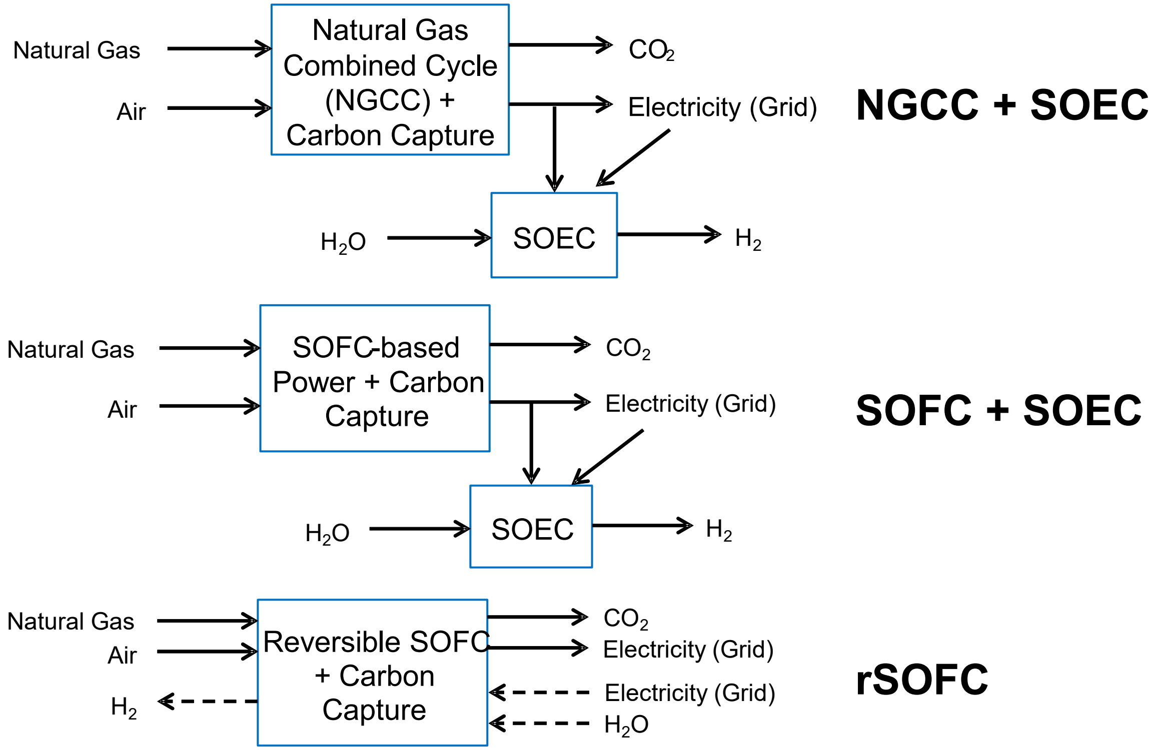
- **Integrated Energy Systems:** Eslick, Noring, Susarla, Okoli, Allan, Wang, Ma, Zamarripa, Iyengar, Burgard, Technoeconomic Evaluation of Solid Oxide Fuel Cell Hydrogen-Electricity Co-generation Concepts (DOE/NETL-2023/4322).
- **Costing Methodology:** Theis, Quality Guidelines for Energy System Studies – Cost Estimation Methodology for NETL Assessments of Power Plant Performance (NETL-PUB-22580).
- **NGCC:** Schmitt, Leptinsky, Turner, Zoelle, White, Hughes, Homsy, Woods, Hoffman, Shultz, and James. Cost And Performance Baseline for Fossil Energy Plants Volume 1: Bituminous Coal and Natural Gas to Electricity (DOE/NETL-2023/4320).
- **SOFC:** Iyengar, Noring, Mackay, Keairns, and Hackett. Techno-economic Analysis of Natural Gas Fuel Cell Plant Configurations (DOE/NETL-2022/3259).
- **SMR & ATR:** Lewis, McNaul, Jamieson, Henriksen, Matthews, White, Walsh, Grove, Shultz, Skone and Stevens, Comparison of commercial, state-of-the-art, fossil-based hydrogen production technologies (DOE/NETL-2022/3241).

High Level Block Flow Diagrams

- Compare optimized IES to stand-alone "competitive" systems
- Evaluate dispatchability in context of real energy markets

"Baseline Systems"– i.e., the competition





Time Permitting: H_2 Storage will also be considered.

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Design and Costing Basis*

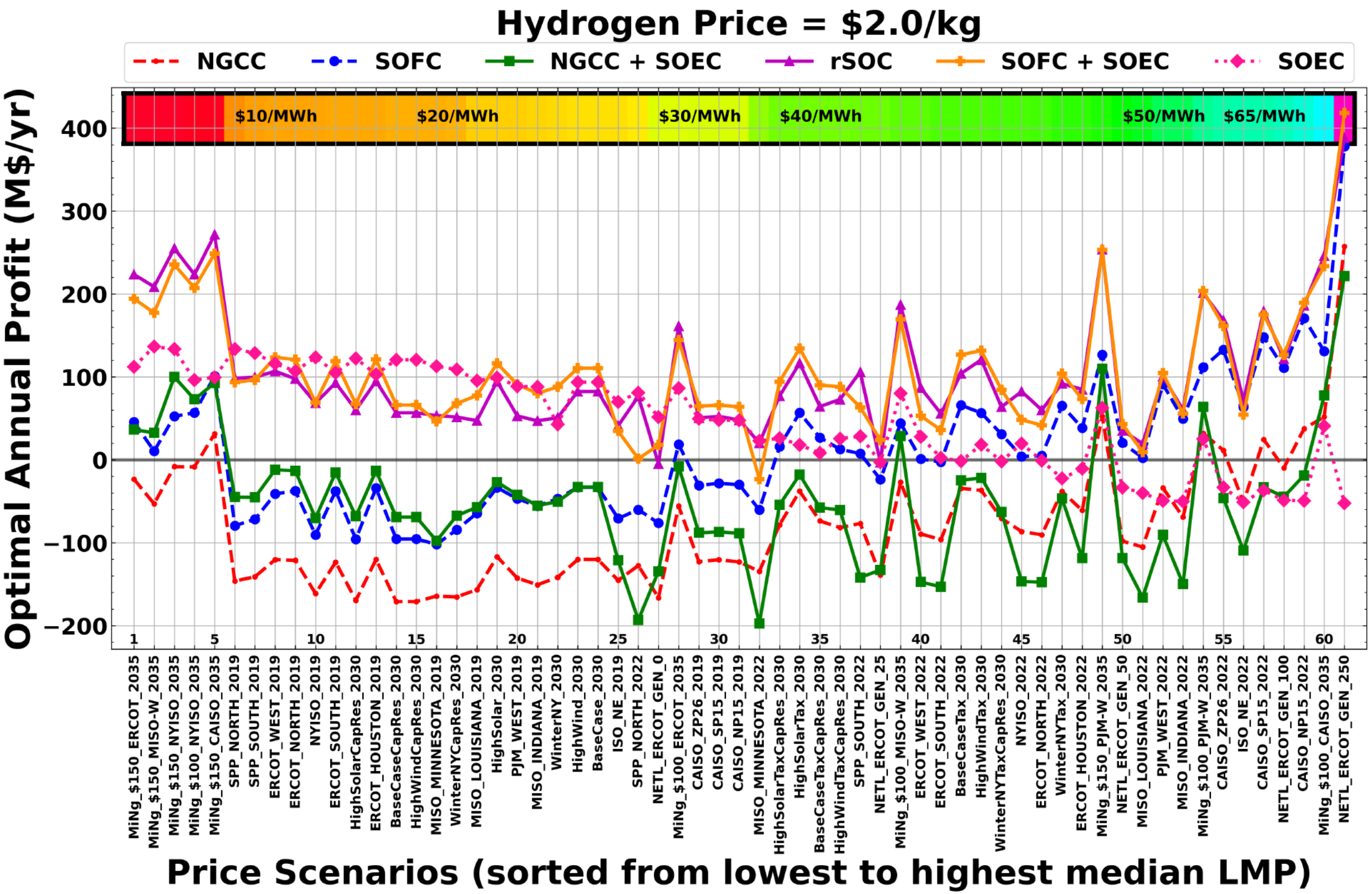
- Greenfield Plants, Midwestern US, 2018 $'s
- Hydrogen: 6.479 MPa, < 10 ppm H_2O
- All systems designed to capture > 97% CO_2
- 100% capacity factor**

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

- SOFC: $225/kW stack cost+
- SOEC: $105/kW stack cost
- Stack degradation rate: 0.2% / 1000 hr (~7 yrs stack life)+

* Theis, Quality Guidelines for Energy System Studies – Cost Estimation Methodology for NETL Assessments of Power Plant Performance, February 2021, (NETL-PUB-22580)
** Major assumption that process-market optimization allows us to relax.
+ Iyengar, Noring, Mackay, Keairns, and Hackett. Techno-economic Analysis of Natural Gas Fuel Cell Plant Configurations (DOE/NETL-2022/3259).

Compiled Results from Integrated Process/Market Optimization



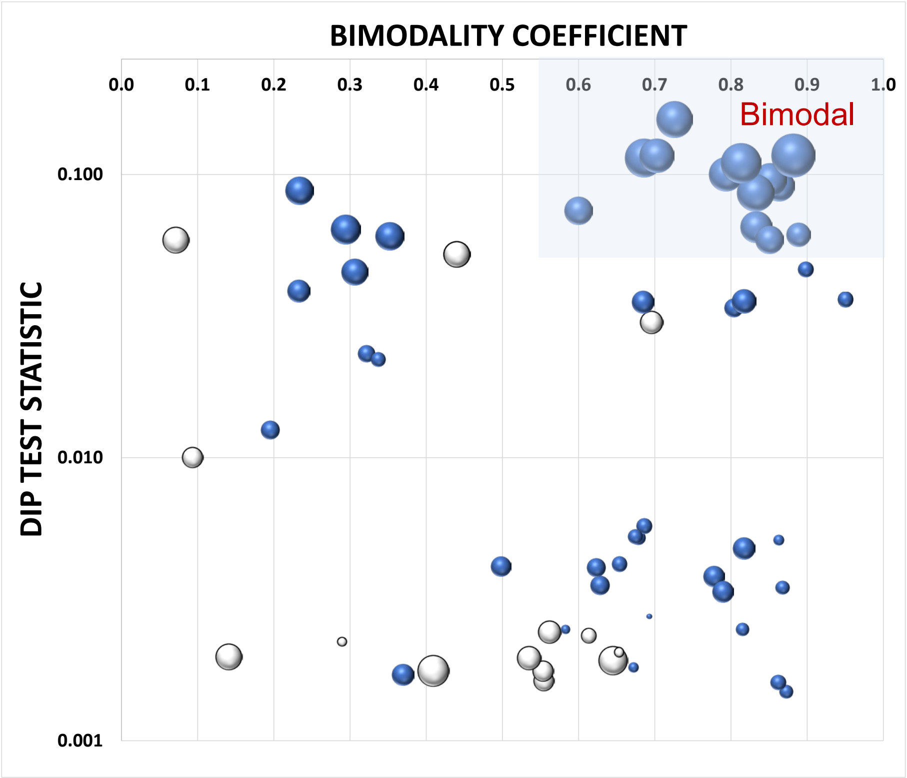
Key Conclusions

% 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.

Bubble Size = Value of Integration:
Annual Profit from SOEC+SOFC –
Max (Annual Profit from SOEC, Annual Profit from SOFC)



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

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