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Institute for the Design of Advanced Energy Systems

IDAES Integrated Platform for Multi-Scale Modeling and Optimization

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September 18, 2024

IDAES Overview

- IDAES is an open-source, equation-oriented software platform, written in Pyomo, that enables the design and optimization of multi-scale, dynamic, interacting technologies and systems.

- Goal**:** Accelerate design & deployment of integrated power, H_2, and industrial processes to support broad decarbonization and emerging R&D priorities.

- 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 Leverage IDAES

Collaboration	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 FE-30*	National Energy Technology Laboratory; Berkeley Lab; Sandia National Laboratories; Carnegie Mellon; West Virginia University; University of Notre Dame; Georgia Tech
WaterTAP	Water Purification *EERE via NAWI & IEDO*	National Energy Technology Laboratory; Berkeley Lab; NREL Transforming ENERGY; Oak Ridge National Laboratory

IDAES Integrated Platform

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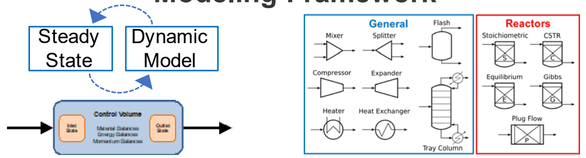
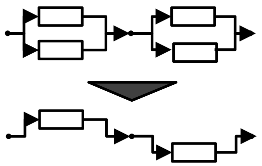
Modeling Framework



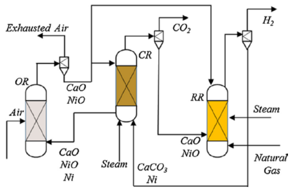
Hierarchical - Steady-State & Dynamic - Model Libraries

Conceptual Design

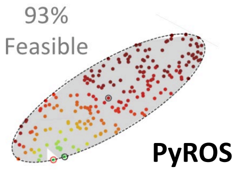


PYOMO GDP

Plant Design Process Optimization



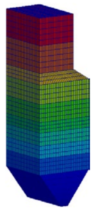
Uncertainty Quantification Robust Optimization



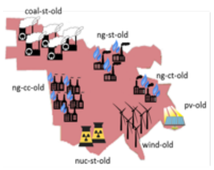
AI/ML Surrogate Modeling

ALAMO a black-box modeling tool

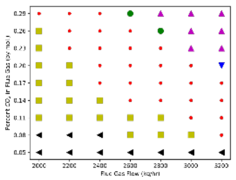
PySMO



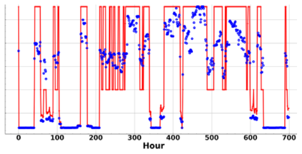
Infrastructure Planning of Reliable Carbon Neutral Power Systems



Process Family Design

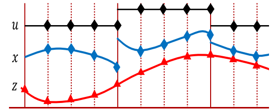


Process/Market Co-Optimization



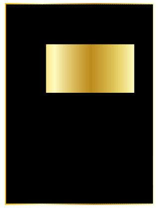
Process Operations Dynamics & Control

caprese



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

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



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

- **Diagnostics, scaling, and visualization advances**
  - Tomorrow, 8:30 AM, Scaling and Diagnostics
  - Poster, Model Diagnostics for EO Models: Roadblocks and Path Forward
  - Tomorrow, 11:30 AM, IDAES Flowsheet Visualizer; WaterTAP/PrOMMiS GUI's

- **AI/ML approaches to improving solution algorithms**
  - Tomorrow, 4:00 PM, AI/ML Approaches to MIPs

- **Infrastructure planning of reliable & carbon-neutral power systems**
  - Today, 4:00 PM, Expansion Planning of Reliable & Carbon Neutral Power …
  - Poster, Optimization Model and Solution Strategy for Infrastructure Planning …
  - Tomorrow, 4:30 PM, Flexible Environments for Generator and Transmission Planning (GTEP) Analysis

IDAES New Capability Development

- **Integrating manufacturing considerations into process design**

- **Integrated process market optimization of power and H_2 systems**

- **Dynamics, control, health modeling & optimization of power & H_2 systems**

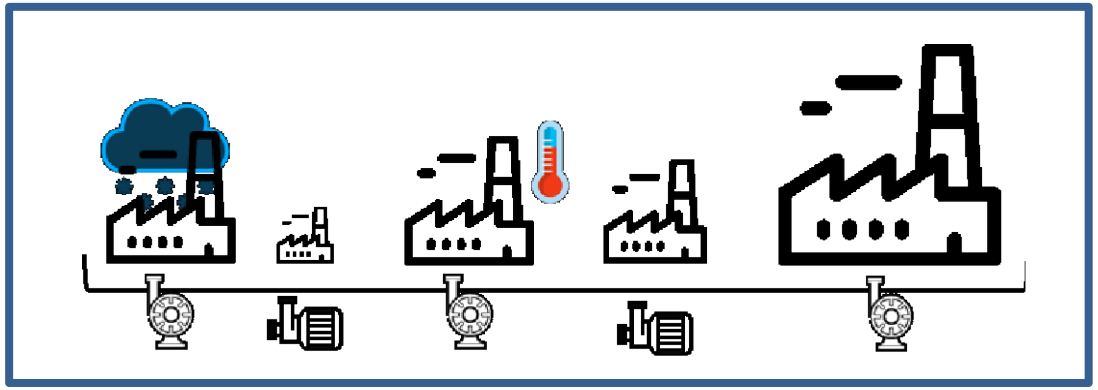
Integration of Manufacturing Considerations into Process Family Design

Objective

Develop a framework for simultaneously designing a family of process variants with different design requirements, while simultaneously optimizing the use of shared sub-components/unit operations.

Why does this matter?

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 # of each of the units)



Design a family of processes over a range of requirements

⇅

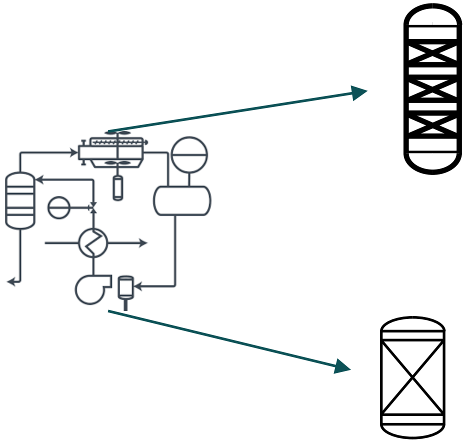
Simultaneously design a platform of shared sub-components

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

Case Study: MEA Carbon Capture

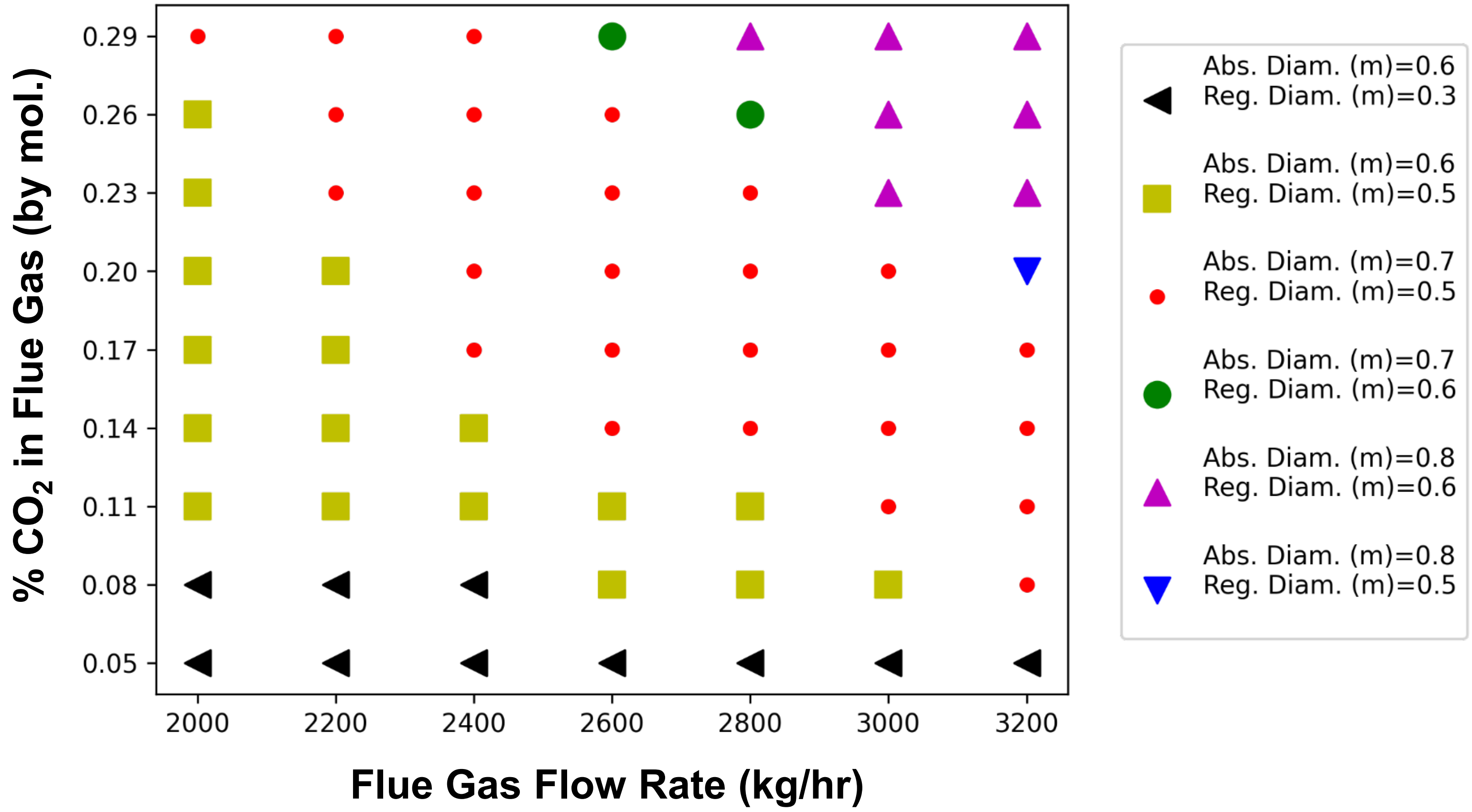
Successfully designed 63 carbon capture systems using only 3 optimally designed absorbers & strippers

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%**

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

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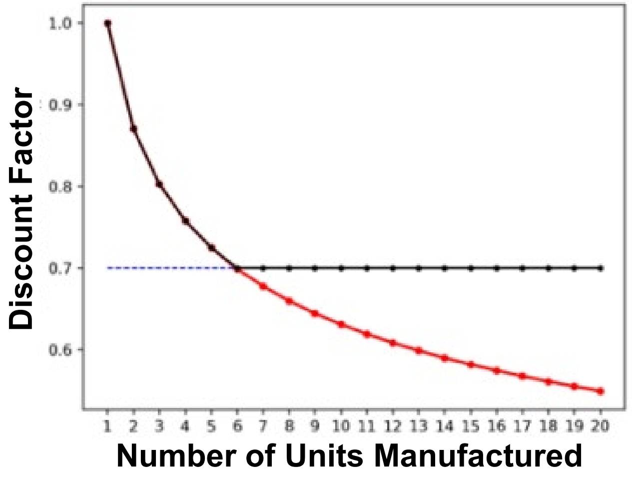
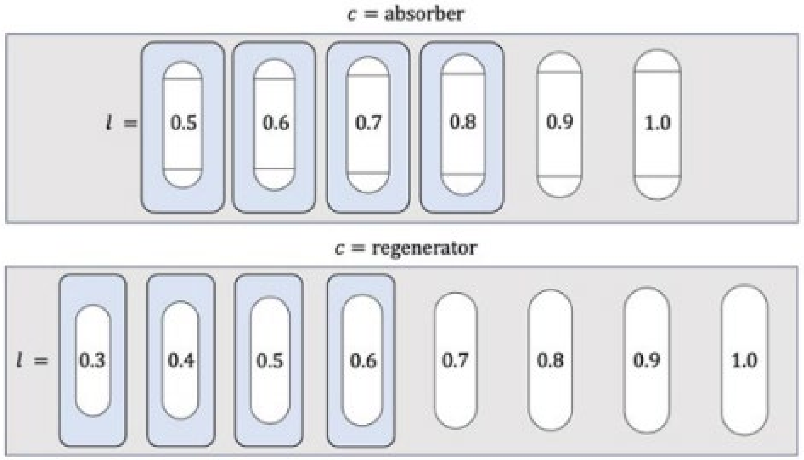
Recent Advances

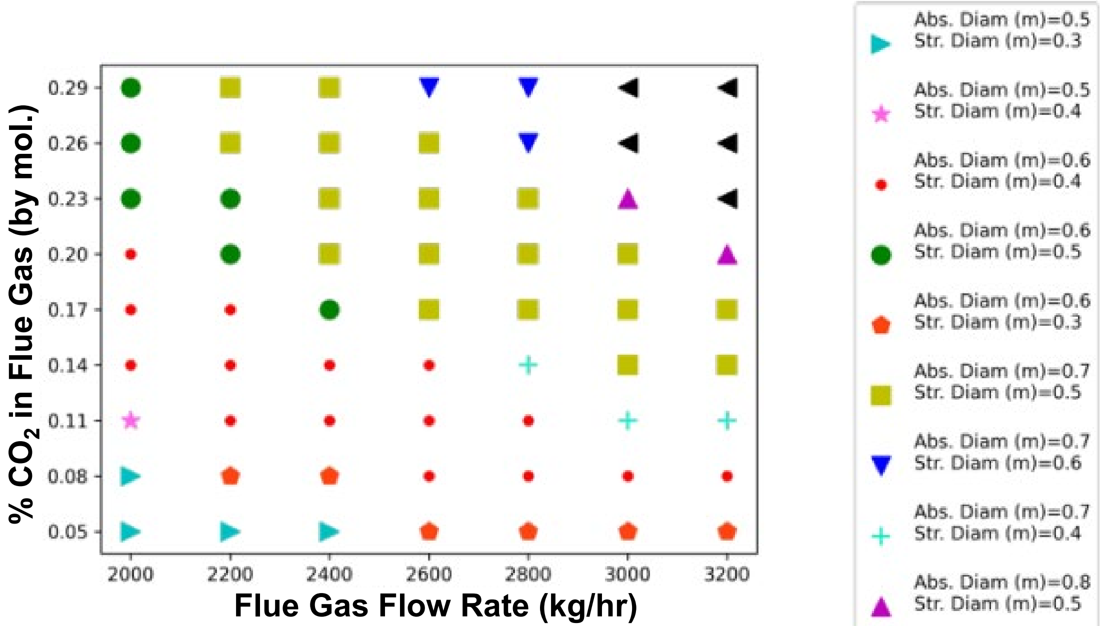
- Improved formulation explicitly includes economies of numbers
  - User no longer needs to specify the size of the platform
  - Optimizes both the number and characteristics of common components



- 4 unique absorber & stripper sizes led to a 26.8% capital cost savings

Case Study: MEA Carbon Capture



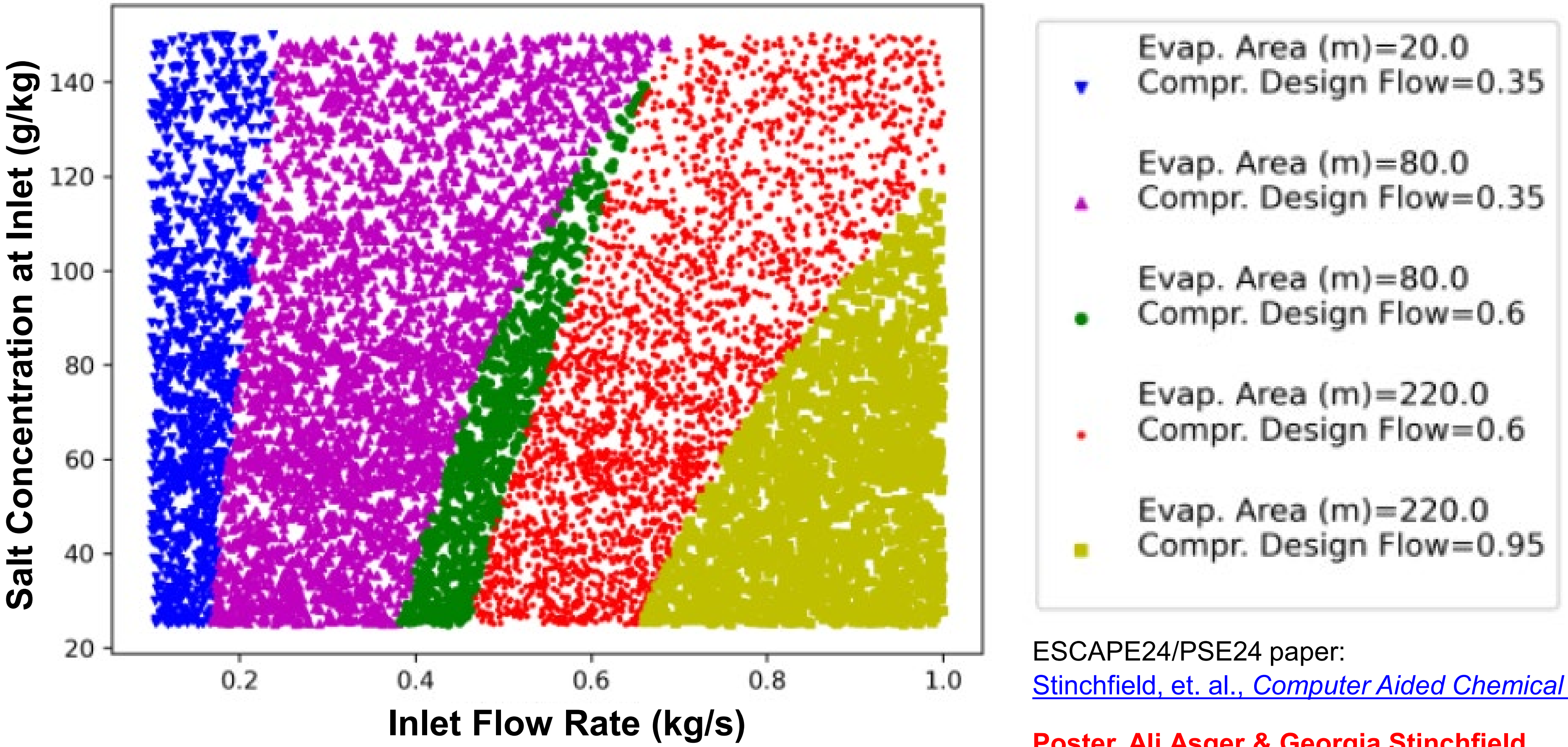


FOCAPD paper:
Stinchfield et. al., *Systems & Control Transactions*, 2024

Recent Advances

- Decomposition approach enabled simultaneous design of 10,000 variants!

Case Study: Water Desalination



ESCAPE24/PSE24 paper:
Stinchfield, et. al., *Computer Aided Chemical Engineering*, 2024

Poster, Ali Asger & Georgia Stinchfield

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IDAES New Capability Development

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

Integrated Process Market Optimization of Power and H_2 Systems

Objective

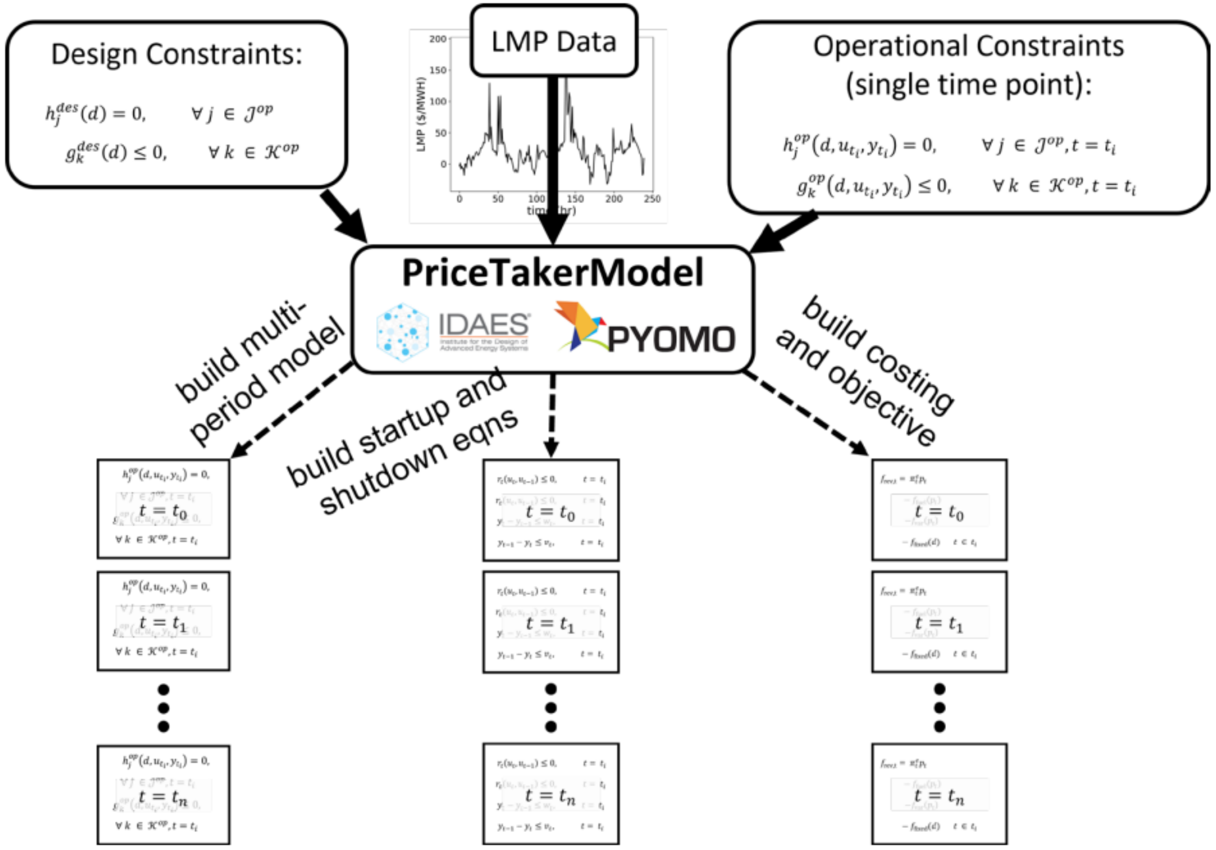
Develop a framework for quantitatively evaluating the value propositions of integrated energy systems in several electricity markets.

Why does this matter?

- Allows meaningful and direct comparisons of IES technology options when traditional metrics (e.g., LCOE, LCOH, cost of capture) are not fully sufficient
- Useful for setting R&D performance targets

Recent Accomplishment

- Streamlined workflow reduces set-up time from months to days.



FOCAPD paper:
[Laky, et. al., *Systems & Controls Transactions*, 2024]

Tomorrow, 9:30 AM, Multi-Period Optimization for Process Design and Market Integration

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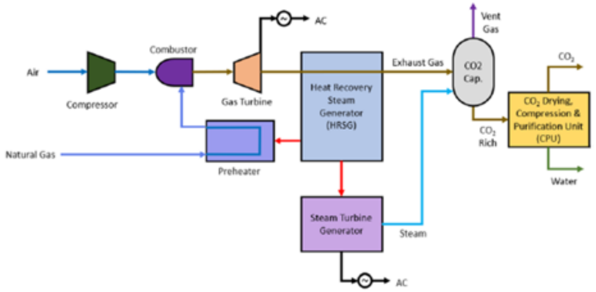
Demonstrating the Value Proposition of Flexible Power/H_2

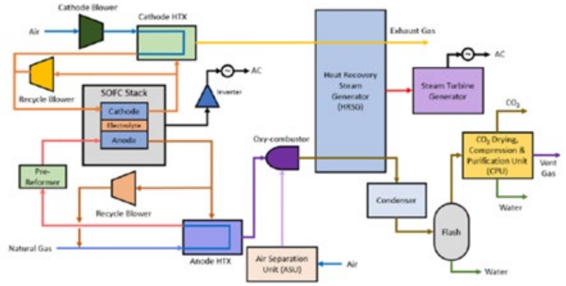
Fuel = Natural Gas
CO_2 capture > 97%

Baseline Systems Single Product

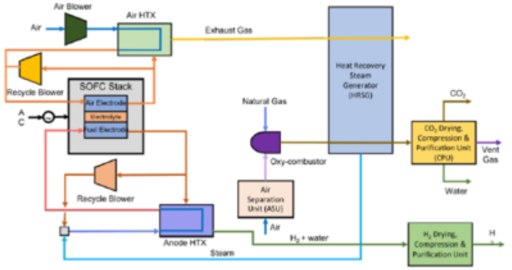
Standalone Natural Gas Combined Cycle (NGCC)
Power Only



Standalone Solid Oxide Fuel Cell (SOFC)
Power Only



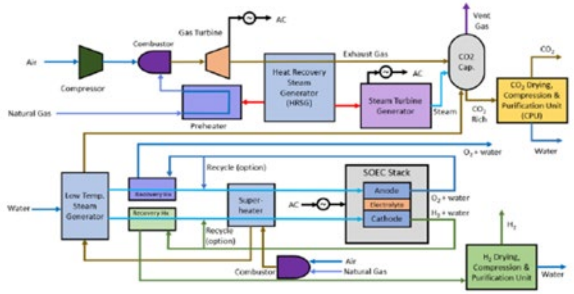
Standalone Solid Oxide Electrolyzer Cell (SOEC)
Hydrogen Only



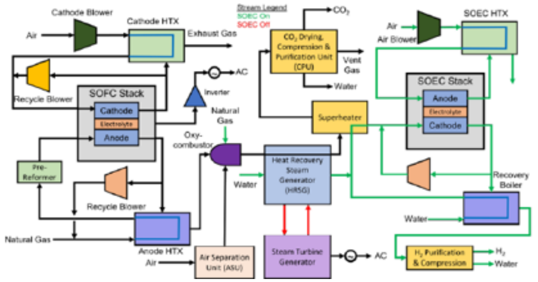
Are there plausible electricity market scenarios where an integrated system makes sense?
If so, which system is the best?

Integrated Systems Multi-Product

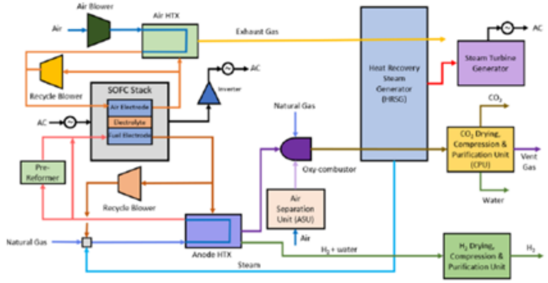
NGCC + SOEC
Power, Hydrogen, Coproduction



SOFC + SOEC
Power, Hydrogen, Coproduction



Reversible Solid Oxide Cell (rSOC)
Power, Hydrogen



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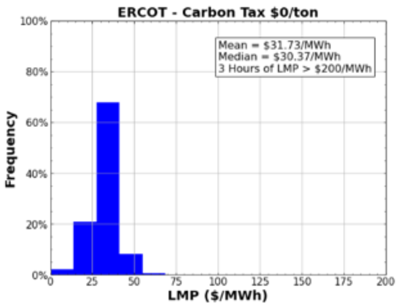
Eslick, et. al., DOE/NETL-2023/4322

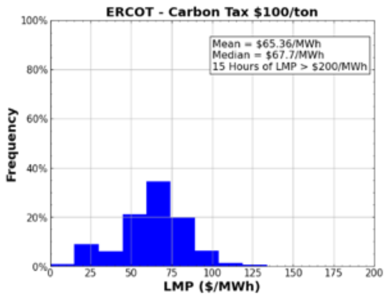
Analysis of Flexible Power and H_2 Systems

- **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

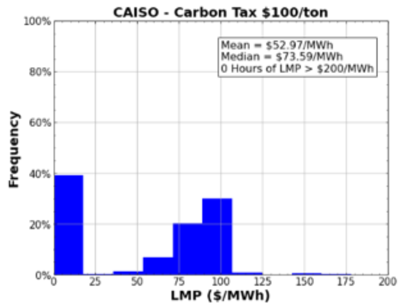
Data sets cover very broad range of potential scenarios



Low Electricity Prices



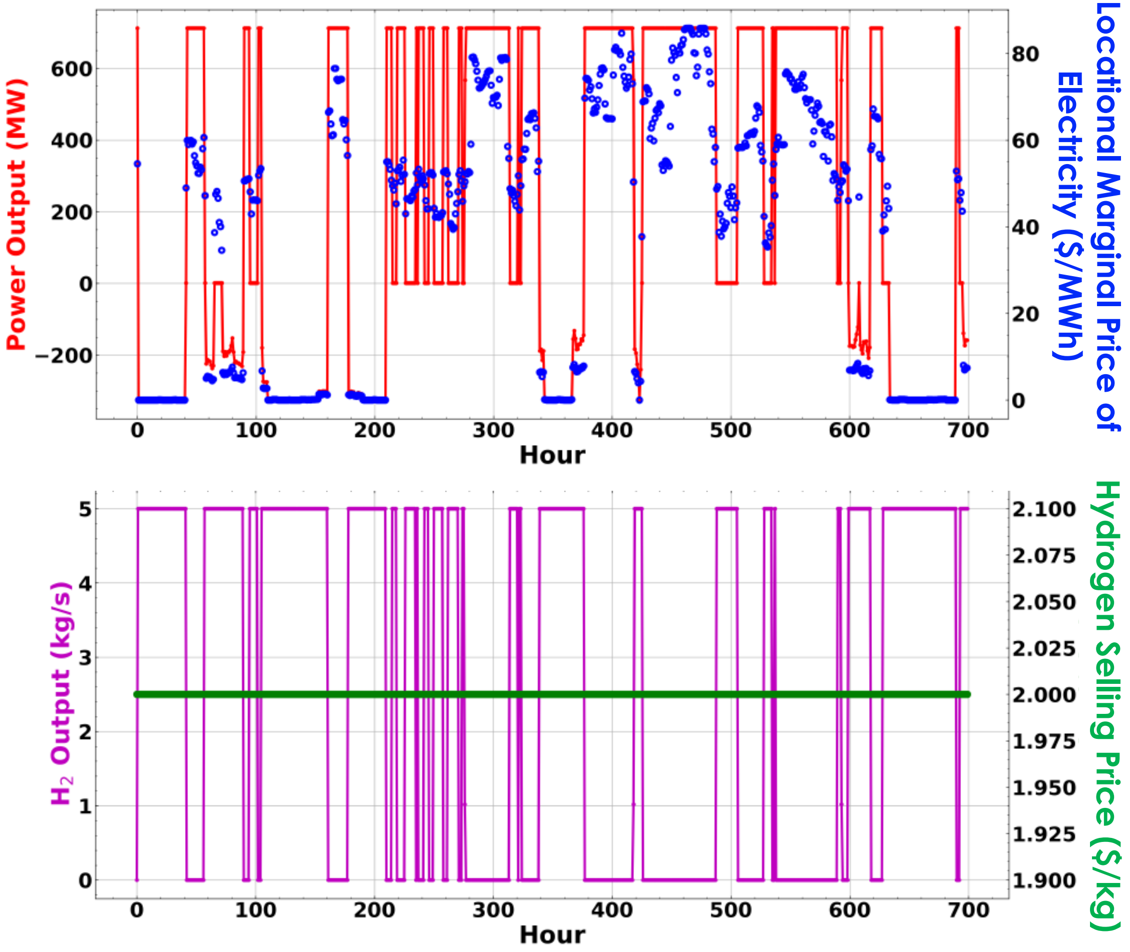
High Electricity Prices



Bimodal (e.g., high VRE)

Optimize IES Operation

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



Flexible Power/H_2 Systems Outperform Single Product Systems

% of Electricity Market Scenarios with Positive Annualized Profit

CO_2 Capture > 97%

	H_2 Selling Price			
Process Concept	**\$1.5/kg**	**\$2.0/kg**	**\$2.5/kg**	**\$3.0/kg**
NGCC	○ 13%			
SOFC	◑ 54%			
SOEC	◑ 49%	◕ 74%	● 87%	● 98%
NGCC + SOEC	○ 11%	○ 16%	◑ 62%	◕ 80%
rSOC	◕ 77%	● 97%	● 100%	● 100%
SOFC + SOEC	◕ 79%	● 98%	● 100%	● 100%

Laky, et. al., 2024, *paper under review*

Poster, Daniel Laky

- Integrated power/H_2 systems are far more robust to electricity market assumptions.

There is a compelling value proposition!

if …

- They can safely switch between operating modes without causing excessive degradation over long-time operation.

IDAES New Capability Development

- Integrating manufacturing considerations into process design
- Integrated process market optimization of power and H_2 systems
- Dynamics, control, health modeling & optimization of power & H_2 systems

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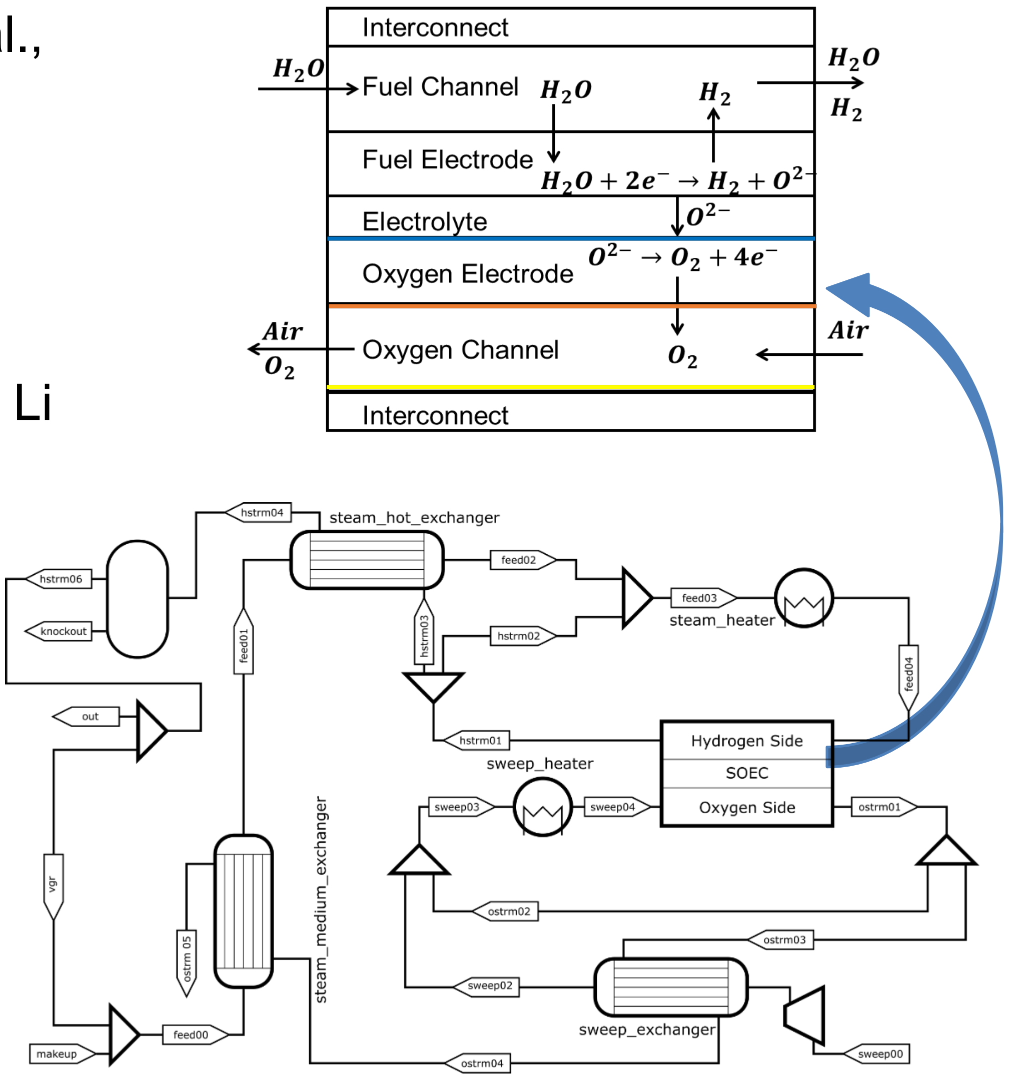
Dynamic Model of SOC-based System for Mode-Switching

- **SOC dynamic model** (Bhattacharyya et al., 2007, Li et al., 2024)
  - 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, Li et al., 2024)
  - 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

- Bhattacharyya et al., Chem Eng Sci, 62, 4250-4267 (2007).
- Allan, D.A., et al., In Proc. FOCAPO/CPC (2023).
- Li M, Allan D A, Dinh S, Bhattacharyya D, Dabadghao V, Giridhar N, Zitney S E, Biegler L T, “NMPC for mode-switching operation of reversible solid oxide cell systems”, e18550, 1-12, AICHE Journal, 2024

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Chemical Degradation

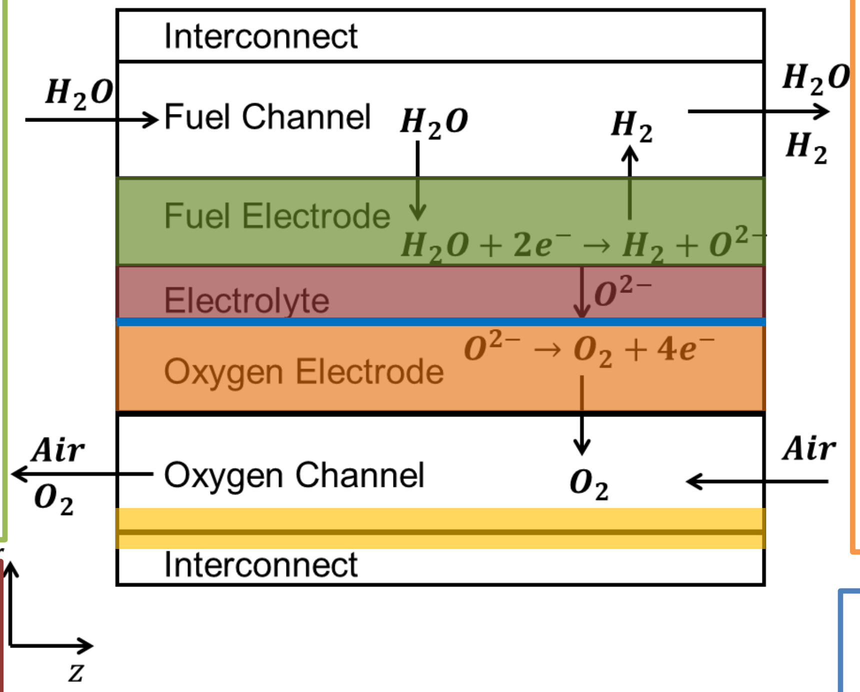
SOEC Microstructure Chemical Degradation Modeling

Fuel electrode nickel (Ni) agglomeration

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

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

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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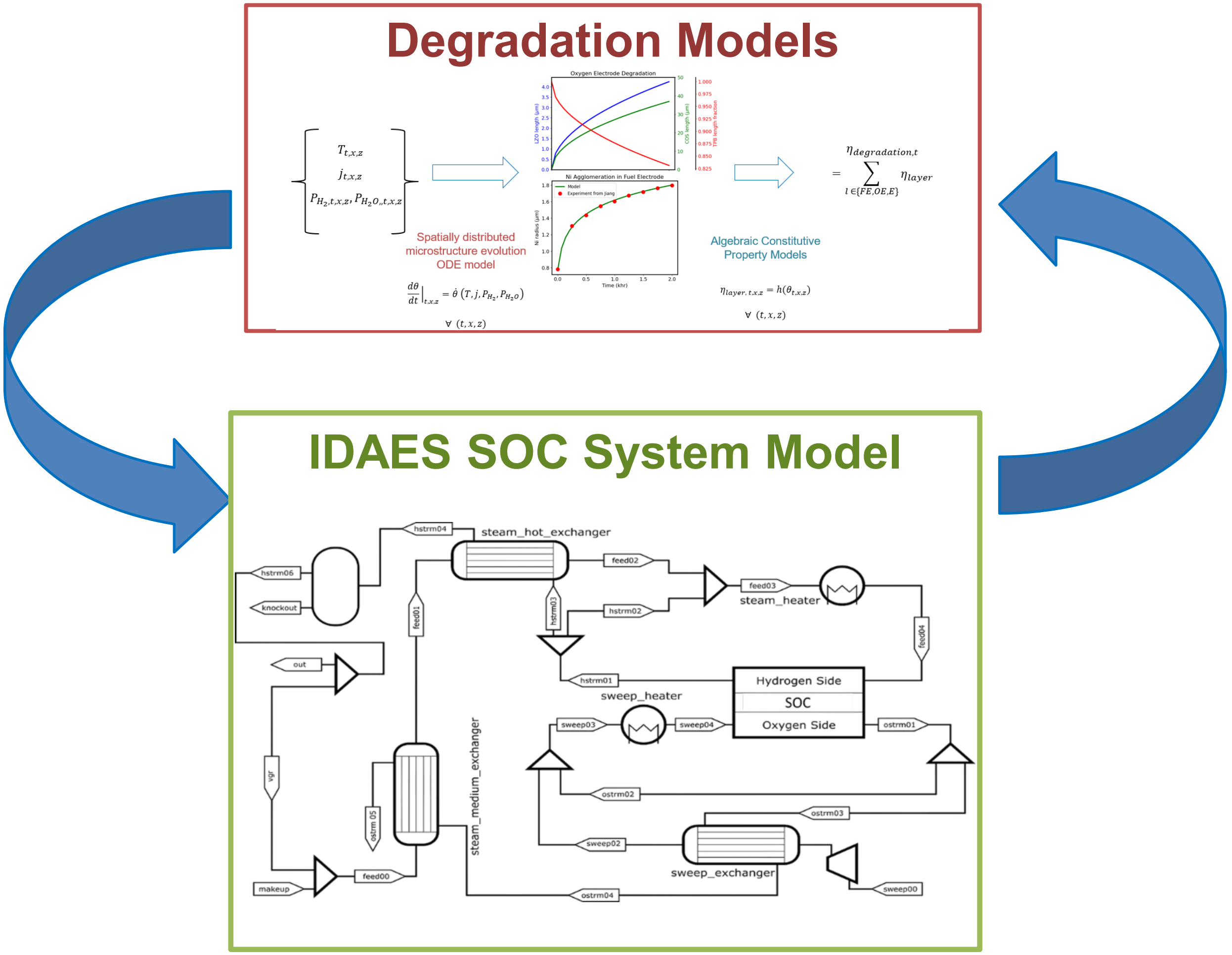
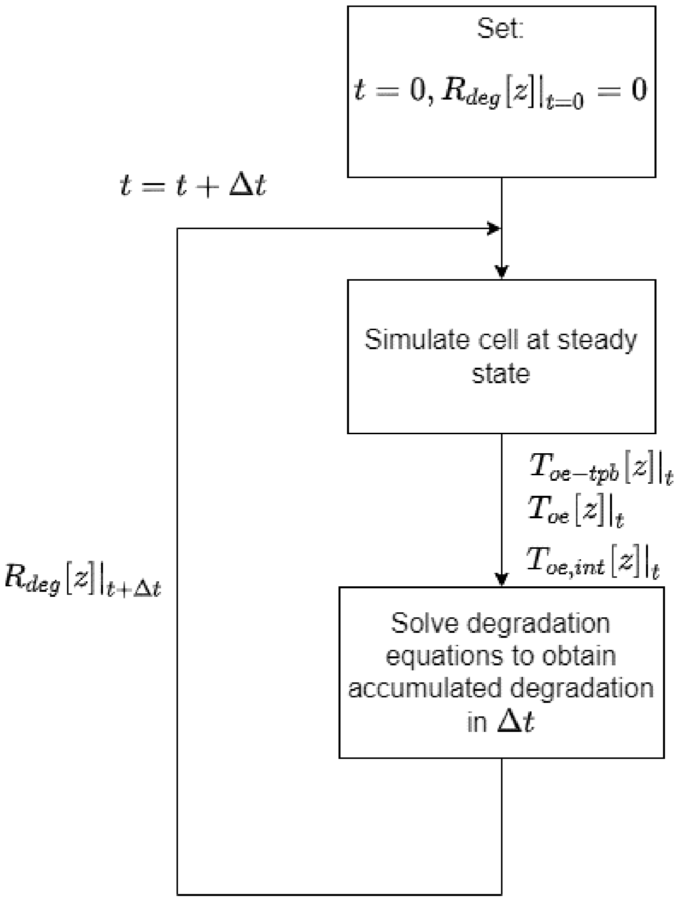
Giridhar N, Zitney S E, Allan D, Li M, Biegler L T, Bhattacharyya D, "Optimal Operation of Solid-Oxide Electrolysis Cells Considering Long-Term Chemical Degradation", 319, 118950, *Energy Conversion and Management*, 2024

Optimizing Multi-Scale Systems



Quasi-steady state assumption



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Long-Term Economic Optimization of SOEC Systems

Economic Considerations

Target operating costs

Counteract efficiency losses caused by degradation

$$\text{maximize} \quad \frac{1}{t_f - t_0}\int_{t0}^{tf} \eta_t dt$$

$$\text{where} \quad \eta_t = \frac{HHV(\dot{m}_{H_2,t})}{P_{system,t}}$$

Leave it to market conditions

Capture tradeoffs through the Levelized Cost of H_2 (LCOH)

$$\text{minimize} \quad LCOH$$

$$\text{where } LCOH = \frac{\text{CAPEX} + \text{OPEX} + \text{Energy Costs}}{Lifetime\ H_2\ Production}$$

Target stack replacement costs

Decrease degradation through operating conditions

$$\text{minimize} \quad \Delta\tilde{V}(\theta_{tf})$$

$$\text{where} \quad \theta_{tf} = \theta_{t0} + \int_{t0}^{tf} \dot{\theta}(x, \theta)dt$$

Key decisions

- Operating mode:
  Potentiostatic, Galvanostatic or Flexible
- Stack Replacement Schedule
- Operating conditions within a stack lifetime
- Balance of plant setpoints

Key Results

Electricity Price = 0.03 $/kWh						
Operating Profile	Objective Function	Stack Replacement Schedule (years)	Voltage Degradation Rate (%/khr)	Specific Energy Consumption (kWh/kg H2)	LCOH ($/kg H2)
Galvanostatic Operation	Minimize Terminal Degradation	5	1.22	40.78	2.00
	Maximize Integral Efficiency	2	3.17	35.65	2.29
	Minimize LCOH	5	2.63	38.45	1.93
Potentiostatic Operation	Minimize Terminal Degradation	3	2.83	39.26	2.11
	Maximize Integral Efficiency	2	3.09	35.65	2.30
	Minimize LCOH	3	2.95	35.64	2.05
Flexible Operation	Minimize Terminal Degradation	5	1.15	40.80	1.99
	Maximize Integral Efficiency	3	3.38	36.44	2.02
	Minimize LCOH	5	3.00	38.30	1.92

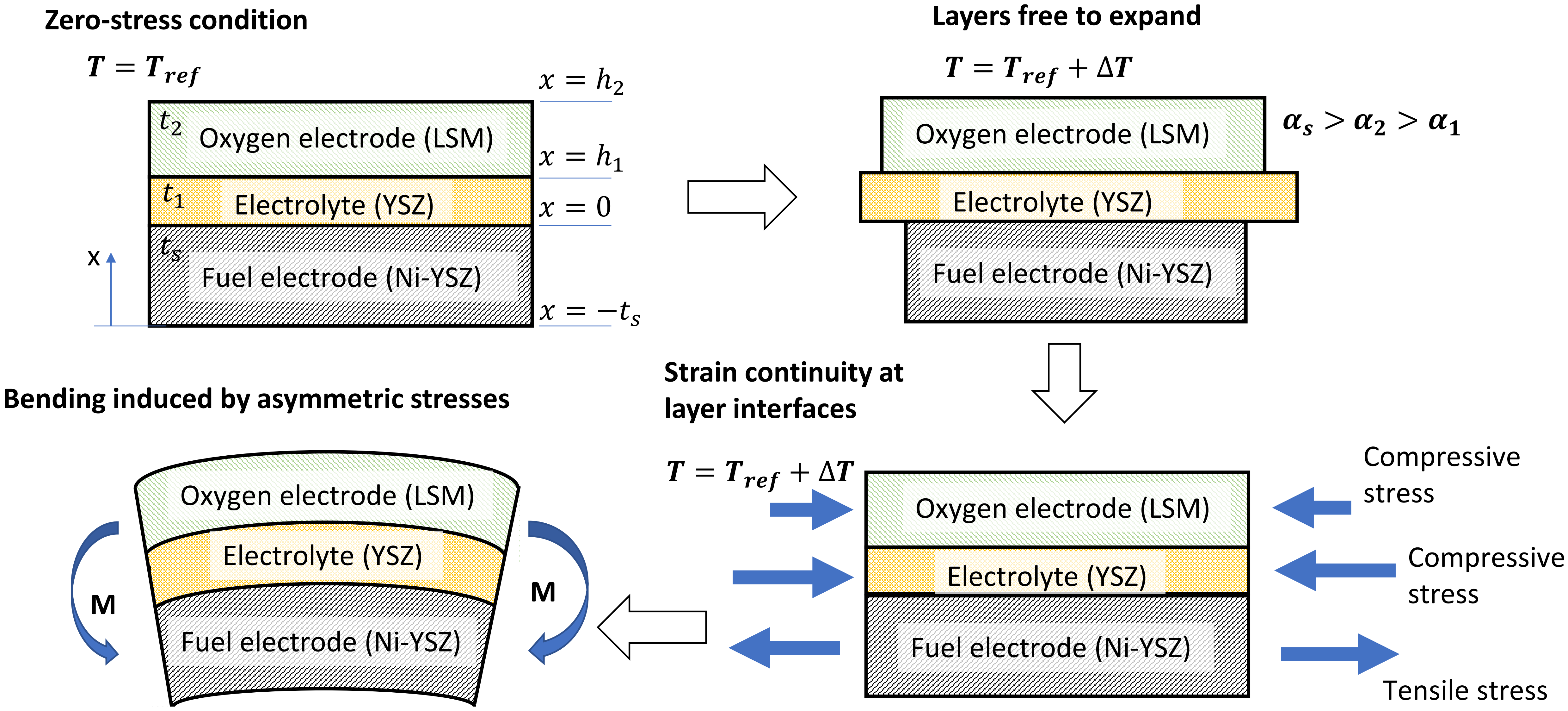
Electricity Price = 0.3 $/kWh					
Operating Profile	Objective Function	Stack Replacement Schedule (years)	Voltage Degradation Rate (%/khr)	Specific Energy Consumption (kWh/kg H2)	LCOH ($/kg H2)
Galvanostatic Operation	Minimize Terminal Degradation	5	1.22	40.78	13.00
	Maximize Integral Efficiency	2	3.17	35.65	11.92
	Minimize LCOH	2.5	3.38	36.02	11.84
Potentiostatic Operation	Minimize Terminal Degradation	3	2.83	39.26	12.51
	Maximize Integral Efficiency	2	3.09	35.65	11.93
	Minimize LCOH	2	3.06	35.64	11.91
Flexible Operation	Minimize Terminal Degradation	5	1.15	40.80	13.01
	Maximize Integral Efficiency	3	3.38	36.44	11.78
	Minimize LCOH	2.5	4.08	35.82	11.78

Giridhar N, Zitney S E, Allan D, Li M, Biegler L T, Bhattacharyya D, "Optimal Operation of Solid-Oxide Electrolysis Cells Considering Long-Term Chemical Degradation", 319, 118950, *Energy Conversion and Management*, 2024

Physical Degradation

Thermal stresses and creep deformation under dynamic operation

Thermal Stress



Dynamic Optimization with Penalty for Deviations from Initial Stress Profile

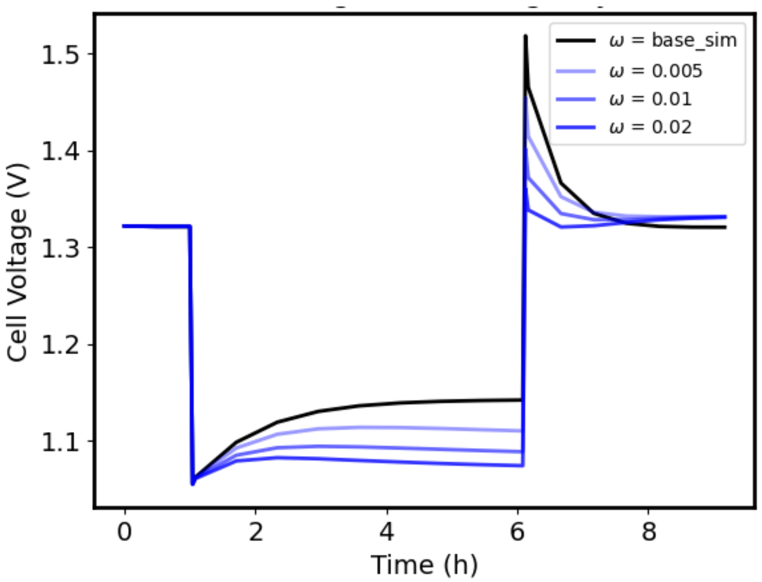
Dynamic Optimization over 1 cycle

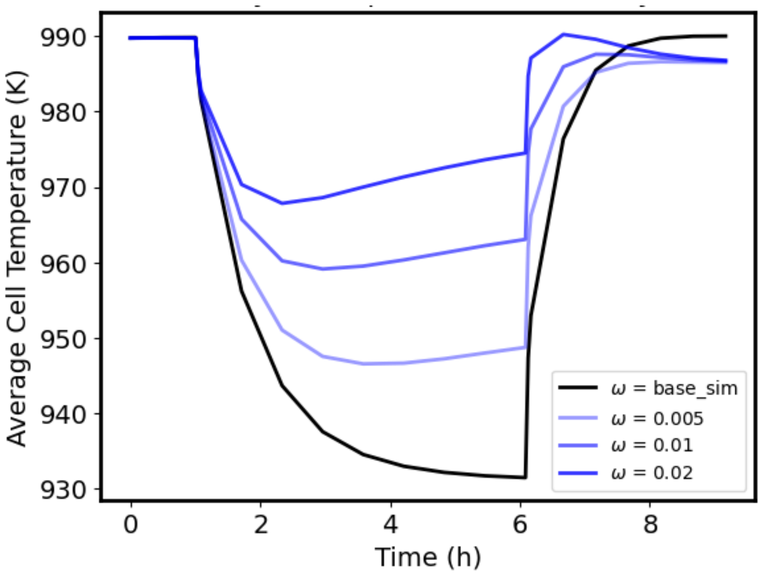
$$max \int_{t_0}^{t_f} \eta_t dt \quad - \omega \int_{t_0}^{t_f} \sum_{x,z} \left(\sigma_{x,z,t} - \sigma_{x,z,0}\right)^2 dt$$

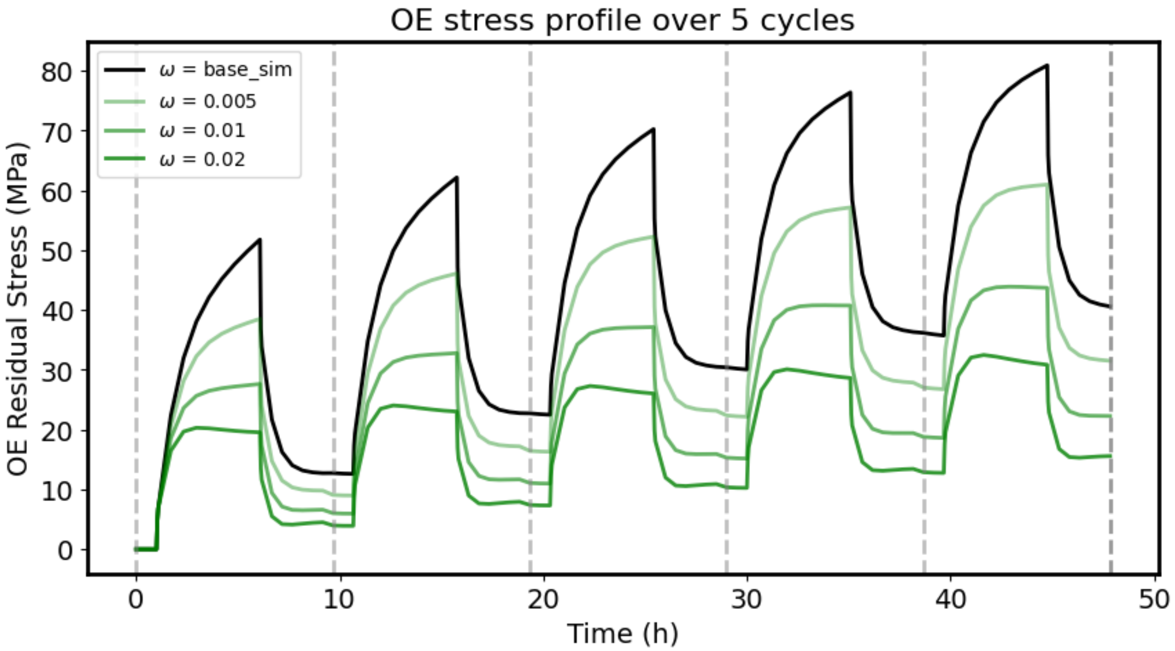
$$st.$$

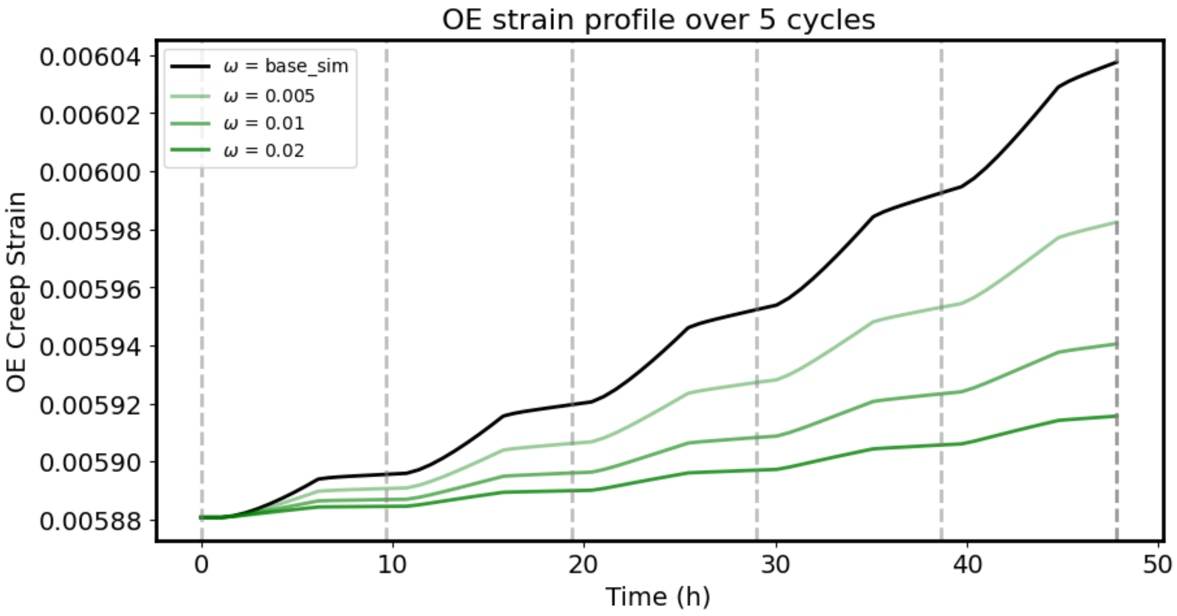
$$h(x) = 0$$

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







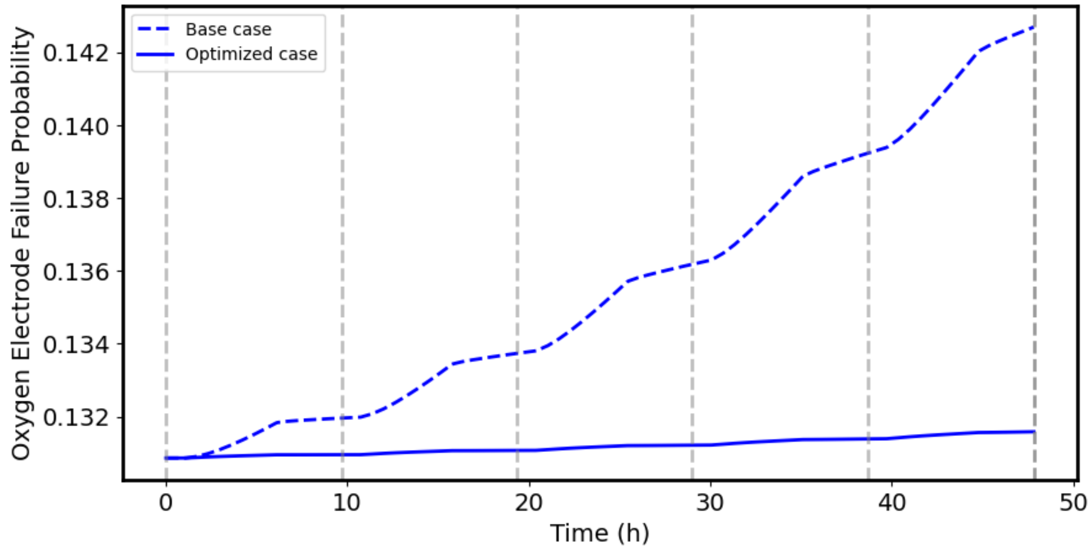


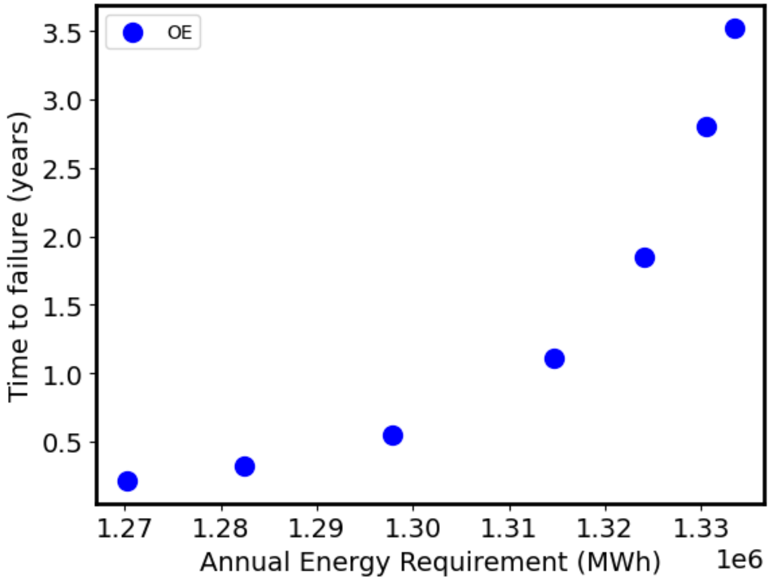
Failure Probability Analysis

Weibull distribution

$$P = 1 - exp\left[-\left(\frac{\epsilon}{\eta}\right)^m \frac{V_f}{V_0}\right]$$

Oxygen Electrode





- Penalizing residual stresses during cycling operation can significantly improve stack lifetimes at the expense of a moderate decrease in operating efficiency.
- The approach can enable stack cycling, reduction in capital expense and improved reliability.

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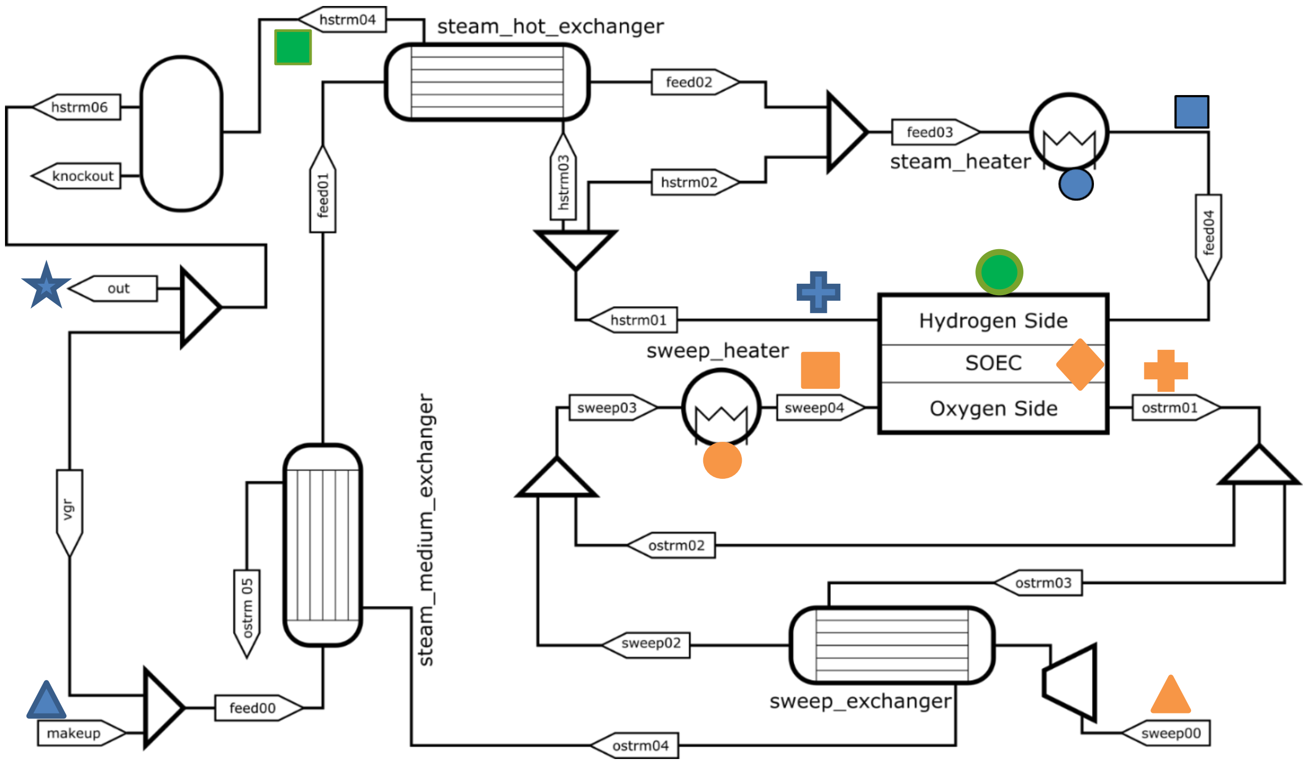
Process Control

Process Control for SOC-based System Mode-Switching

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

$$f_{\text{obj}} = \sum_{i=0}^{N} \rho_{\text{H}_2}\left(y_i - y_i^R\right)^2 + \sum_{i=0}^{N}\sum_{j\in J} \rho_j\left(u_{ij} - u_{ij}^R\right)^2 + \sum_{i=0}^{N}\sum_{k\in K} \rho_k\left(x_{ik} - x_{ik}^R\right)^2$$
$$+ \sum_{i=1}^{N} \rho'\left(v_i - v_{i-1}\right)^2 + \sum_{i=0}^{N}\sum_{z=1}^{z_L} \rho_M \left(\frac{\partial^2 T_{iz}}{\partial z \partial t}\right)^2$$



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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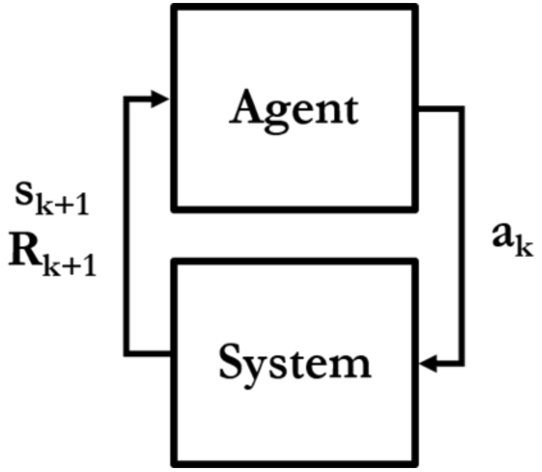
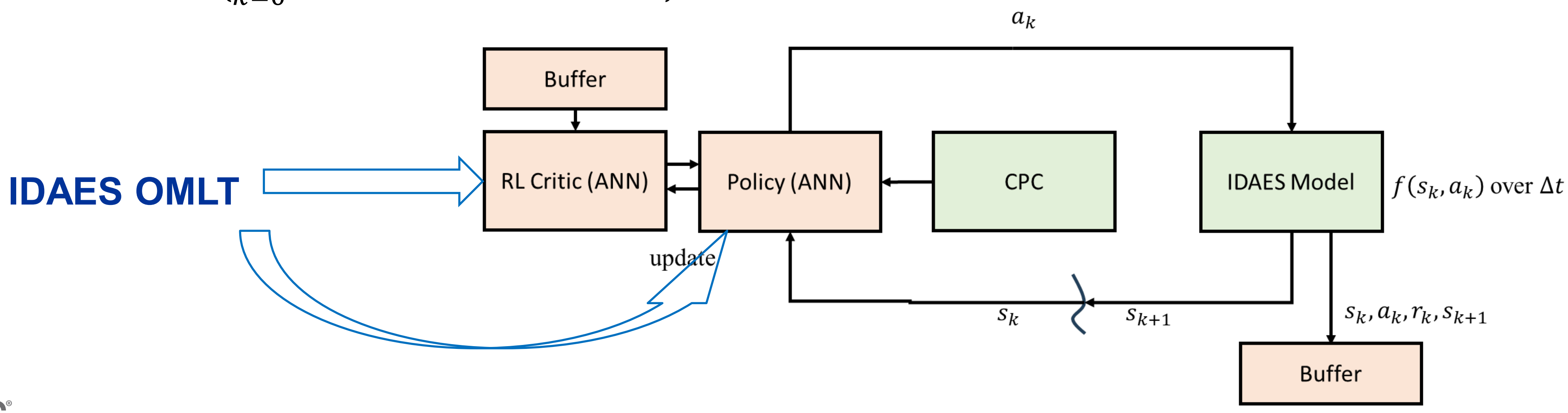
Reinforcement Learning for Process Control

- **Reinforcement learning (RL)** is a machine learning method that learns from active sampling of system performance
- Learning based on a value function and/or a control policy
  - Algorithms with a **fixed policy** – focused on learning a value function given the fixed policy (e.g., Q-Learning, SARSA)
  - Algorithms where **the policy is learned with a value function** – actor-critic methods; parameterized policy and value function used for control
  - General goal is to **maximize expected sum of rewards:**



$$Q^{\pi}(s,a) = E\left\{\sum_{k=0}^{\infty} \gamma^k r_{t+k+1} | s_t = s, a_t = a\right\}$$



Beahr, D., Bhattacharyya, D., Allan, D. A., & Zitney, S. E. (2024). Development of algorithms for augmenting and replacing conventional process control using reinforcement learning. *Computers & Chemical Engineering*, *190*, 108826. https://doi.org/10.1016/j.compchemeng.2024.108826

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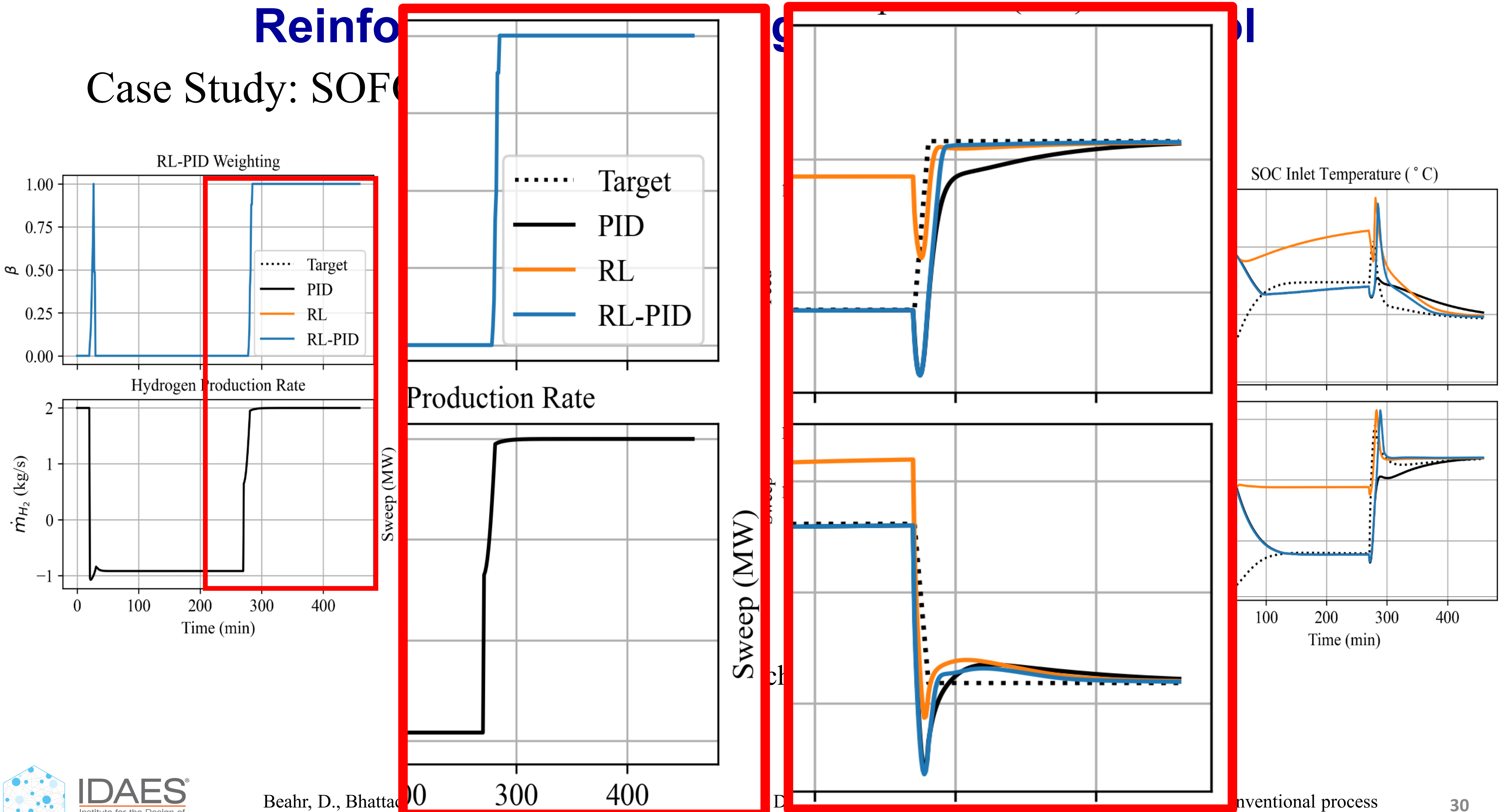
Case Study: SOF(



Beahr, D., Bhattac D nventional process control using reinforcement learning. *Computers & Chemical Engineering*, *190*, 108826. https://doi.org/10.1016/j.compchemeng.2024.108826

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Conclusions

- **Long-term SOEC optimization** considering **chemical degradation** can be used to optimize **stack replacement schedule** and **operating trajectory.**

- **Dynamic optimization** considering **physical degradation** can be used to optimize SOEC operating trajectories to **satisfy spatio-temporal stress constraints** without much sacrifice in the overall efficiency.

- **RL** can **learn** by itself, and from human operators and/or existing conventional controllers and can continuously **adapt** for superior control performance.

- **AI/ML tools in IDAES** can be used by **themselves or hybridized** with rigorous mechanistic models for optimal schedule, design, operation, and decision making.

– Poster: Optimal Schedule, Design, and Operation of Solid Oxide Electrolysis Cell Systems Accounting for Long-Term Performance and Health Degradation (by Nishant Giridhar)

– Tomorrow, 10:00 AM, Dynamic Flowsheeting (by Doug Allen)

Summary

- IDAES is currently supporting several collaborative modeling partnerships aimed at addressing major national and DOE priorities.

- Significant progress has been made towards developing, documenting, and disseminating the next round of foundational capabilities:
  - Advanced diagnostics, scaling, and visualization tools
  - Expansion planning w/ reliability considerations
  - AI/ML approaches to improving MIP solution algorithms
  - Process family design
  - Process/market co-optimization
  - Health modeling, control & dynamic optimization

- IDAES is particularly well-suited to evaluating & designing complex, multi-scale dynamic systems

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