IDAES
Institute for the Design of
Advanced Energy Systems

IDAES Dynamic Modeling, Simulation, and Optimization

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NATIONAL ENERGY TECHNOLOGY LABORATORY
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Motivation: Dynamic Modeling, Simulation, and Optimization

- No plant is truly at steady state
- When optimization is used for design, resulting plant may not be **controllable**
  - Setpoint transition
  - Start up/shut down
- **Dynamic operation** of integrated energy systems (IES) can take advantage of dynamic electricity pricing
- **Equipment degradation** occurs over thousands of hours

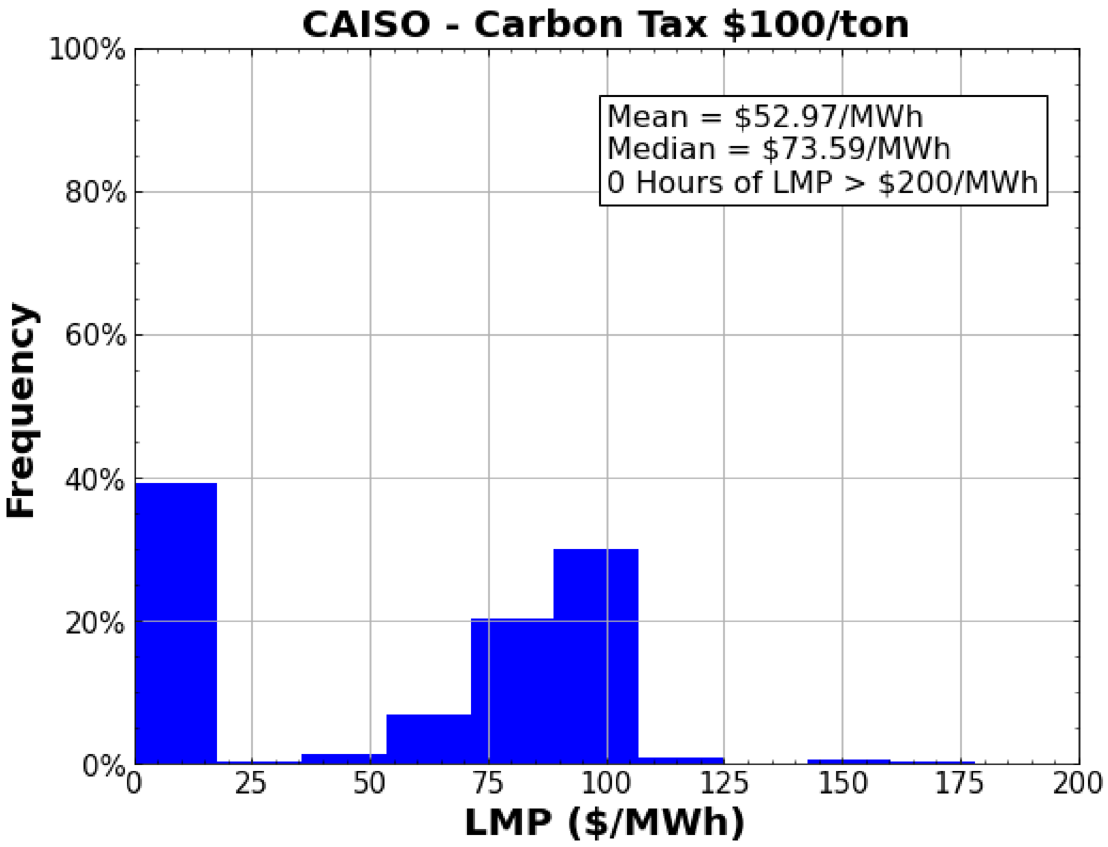
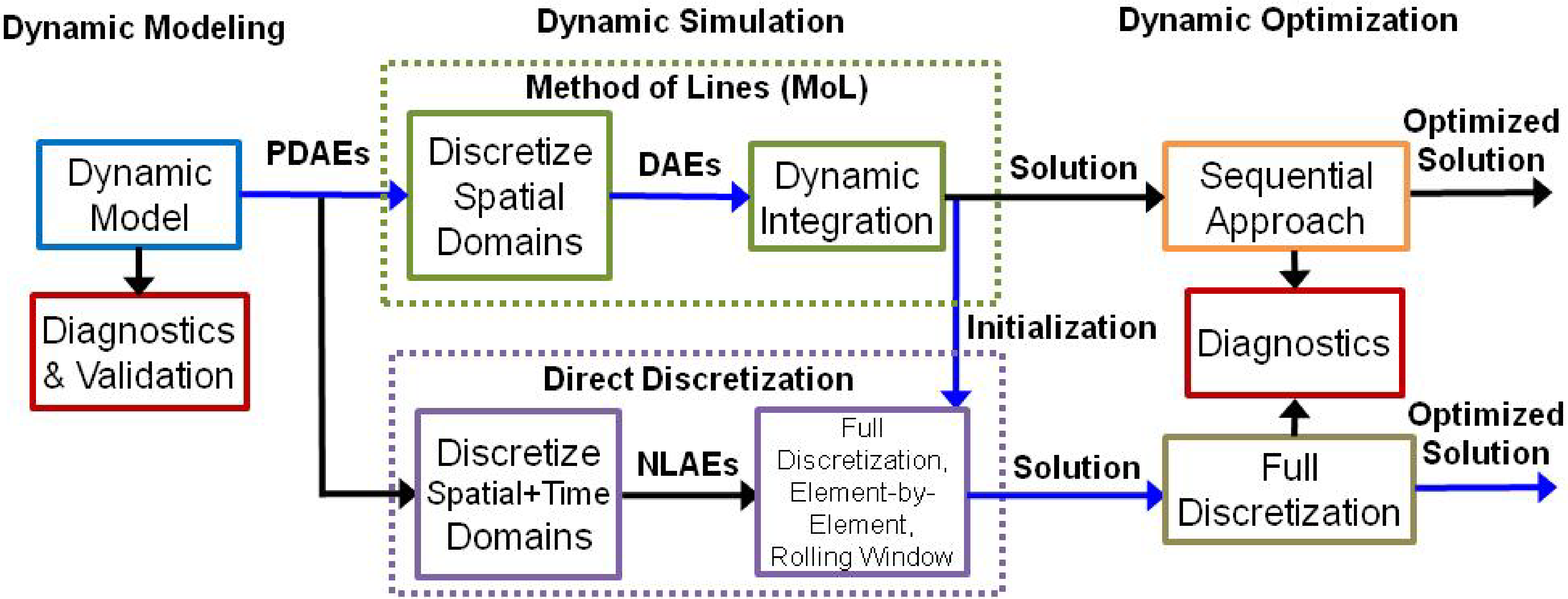


Figure from a presentation by Cortes et al.

(Price Signal Data): Cohen, Stuart; Durvasulu, Venkat (2021): NREL Price Series Developed for the ARPA-E FLECCS Program. National Renewable Energy Laboratory.

IDAES Dynamic Modeling/Simulation/Optimization Workflow



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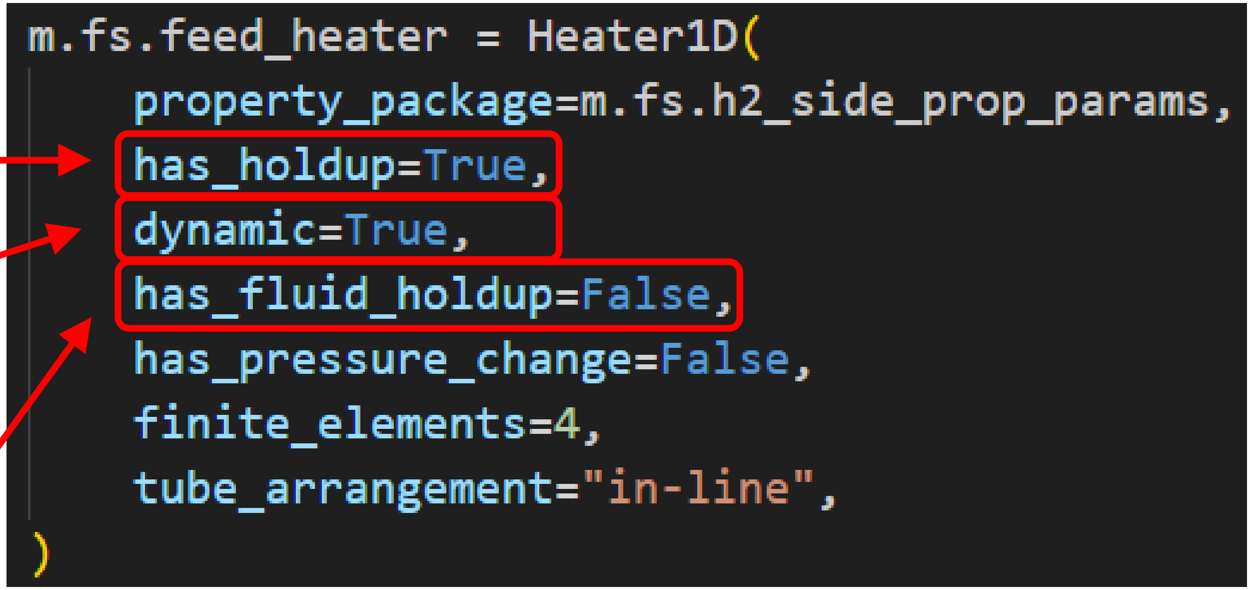
Going from Steady State to Dynamic

- Most models in IDAES feature two config options relative to dynamics:
  - One to generate material and/or energy holdup terms
  - One to create a fully dynamic unit model
- Both must be active for dynamic simulation
- Some models may have additional options for holdup and/or dynamics



```
m.fs.feed_heater = Heater1D(
    property_package=m.fs.h2_side_prop_params,
    has_holdup=True,
    dynamic=True,
    has_fluid_holdup=False,
    has_pressure_change=False,
    finite_elements=4,
    tube_arrangement="in-line",
)
```

Example: Zero-Dimensional Heater

- Default equations:

$$F_{in} = F_{out}$$

$$x_{in,i} = x_{out}$$

$$F_{in}\underline{H}_{in} + Q = F_{out}\underline{H}_{out}$$

Where did the extra equation go?

- Turn on holdup:

$$\left.\begin{aligned} F_{in} &= F_{out} \\ x_{i,in} &= x_{i,out} \\ F_{in}\underline{H}_{in} + Q &= F_{out}\underline{H}_{out} \end{aligned}\right\} \boldsymbol{n_i + 2} \textbf{ equations}$$

$$n_{i,holdup} = \frac{x_i V}{\underline{V}_{holdup}}$$

$$H_{holdup} = \underline{H}_{holdup} n_t$$

- Turn on dynamics:

$$\left.\begin{aligned} \frac{dn_{i,holdup}}{dt} &= F_{in}x_{i,in} - F_{out}x_{i,out} \\ \frac{dH_{holdup}}{dt} &= F_{in}\underline{H}_{in} + Q - F_{out}\underline{H}_{out} \end{aligned}\right\} \boldsymbol{n_i + 1} \textbf{ equations}$$

$$n_{i,holdup} = \frac{x_i V}{\underline{V}_{holdup}}$$

$$H_{holdup} = \underline{H}_{holdup} n_{t,holdup}$$

Stating the Obvious

- Have not determined whether system is liquid or gas yet
- Liquid holdup volume can change with fluid level,
  - Augment system with additional ODE:

$$\frac{dV}{dt} = F_{in}\underline{V}_{in} - F_{out}\underline{V}_{out}$$

- Gases always expand to fill the volume given
  - Augment system with equation of state, like ideal gas law:

$$PV = n_t RT$$

- Dynamics **will expose** modeling shortcuts and inadequacies

Heavy Metal

- We have a dynamic model that solves
- Does it actually capture the dynamics important to us?

> *…the commonly used assumption that wall capacitance may be neglected for liquid exchangers is not valid. For gas exchangers the ratio is at least an order of magnitude larger due to the lower fluid density. Thus, the wall capacitance is expected to completely dominate the dynamics of gas exchangers, and this is in accordance with previous results.* – Mathisen, Morari, and Skogestad, 1994

- We have not even considered metal mass yet.
- All other holdup terms can be ignored for gas phase systems

Mathisen, Knut W., Manfred Morari, and Sigurd Skogestad. "Dynamic models for heat exchangers and heat exchanger networks." *Computers & chemical engineering* 18 (1994): S459-S463.

Revised Dynamic Models

- For liquids, the metal holdup terms augment the liquid thermal holdup

$$\frac{dn_{i,holdup}}{dt} = F_{in}x_{i,in} - F_{out}x_{i,out}$$

$$n_{i,holdup} = \frac{x_i V}{\underline{V}_{holdup}}$$

$$\frac{dH_{holdup}}{dt} = F_{in}\underline{H}_{in} + Q - F_{out}\underline{H}_{out}$$

$$H_{holdup} = \underline{H}_{Liq}n_t + \hat{H}_{metal}m_{metal}$$

$$\frac{dV}{dt} = F_{in}\underline{V}_{in} - F_{out}\underline{V}_{out}$$

- For gases, we can suppress holdup terms for everything besides the metal

$$0 = F_{in}x_{i,in} - F_{out}x_{i,out}$$

$$\frac{dH_{holdup}}{dt} = F_{in}\underline{H}_{in} + Q - F_{out}\underline{H}_{out}$$

$$H_{holdup} = \hat{H}_{metal}m_{metal}$$

- Problem solved!
- Wait, are metal and gas in thermal equilibrium?

Some Assembly Required

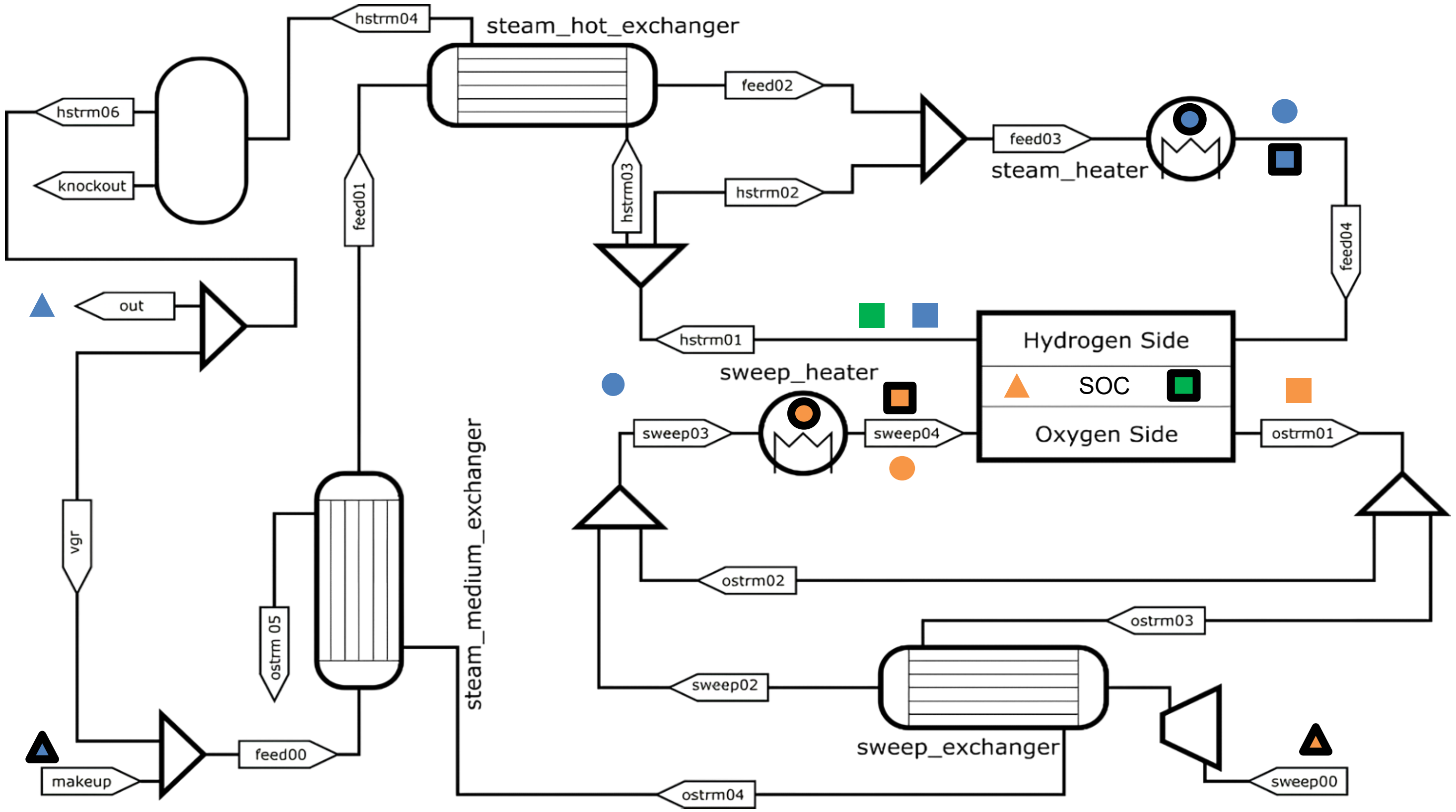
- Many more considerations for dynamics than steady state
  - Heater metal mass and geometry
  - Heat transfer coefficients
- The IDAES framework takes care of many of these considerations with the `StateBlock` and `ControlVolume` classes
  - User still needs to add equations to deal with, e.g., metal mass
- Not every unit model in a dynamic flowsheet needs to be dynamic.
  - Blowers, splitters, and gas mixers should all be steady state elements
- Existing models may accept a `dynamic=True` option, but they do not take these considerations into account
  - The `Heater` model, for example, just creates fluid holdups, which are inadequate for liquids and irrelevant for gases
- Make sure you know **what dynamics are relevant for your use case** before using an off-the-shelf dynamic model

IDAES Dynamic Modeling/Simulation/Optimization Workflow

- **PYOMO DAE**
  - Develop differential algebraic equation (DAE) model
  - Apply diagnostic tools for structural/numerical analysis
- **IDAES**
  - Set some/all unit models to be dynamic
  - PID Controller implemented with anti-windup
- **Dynamic Simulation**
  - Method-of-Lines (MoL) (AMPL/PETSc/TS)
  - Direct Discretization
- **Dynamic Optimization**
  - Full Discretization
  - Can implement nonlinear model predictive control (NMPC)

Case Study: Control of Solid Oxide Cell (SOC)-IES

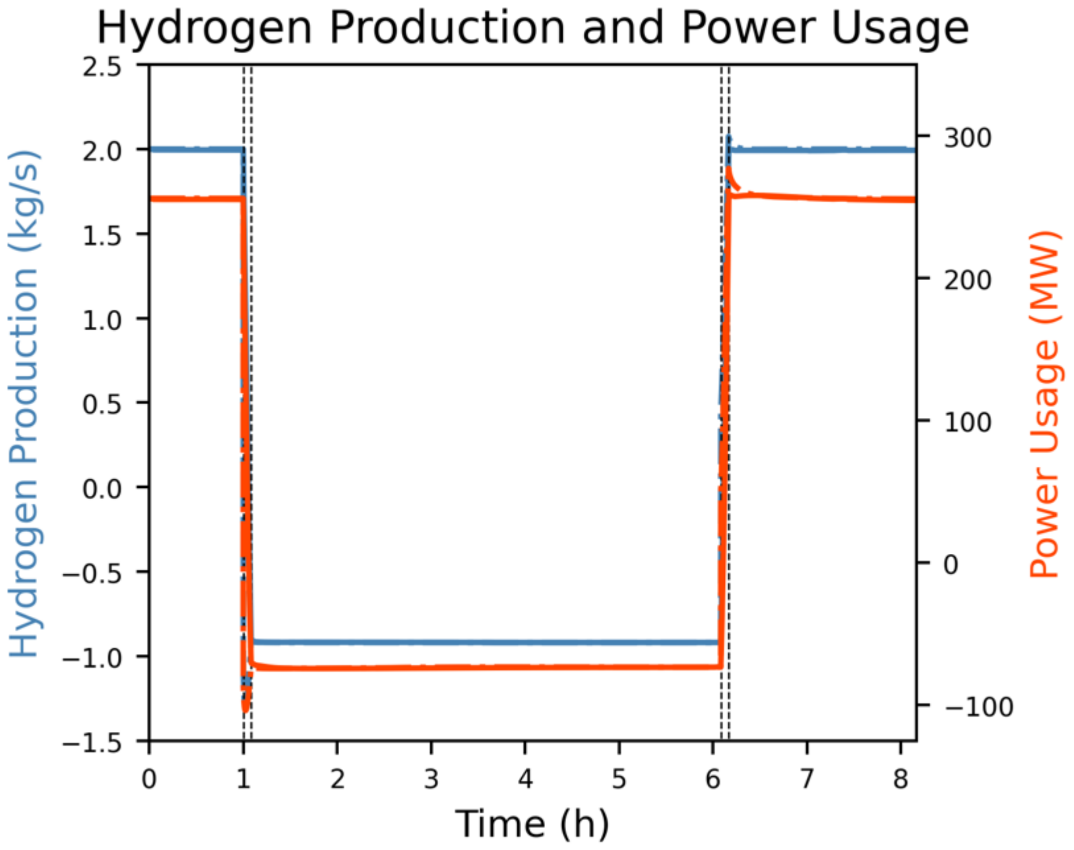
Controller Type	Manipulated Variable (MV)	Controlled Variable (CV)
PI	Cell potential 🟩	SOC fuel outlet H2 mole fraction 🟩
P	Makeup feed rate ▲	Hydrogen production rate ▲
P	Sweep feed rate ▲	SOC stack core temperature ▲
PI (C1I)	Steam heater duty ●	Steam heater outlet temperature ●
PI (C2I)	Sweep heater duty ●	Sweep heater outlet temperature ●
P (C1O)	Steam heater outlet temperature setpoint* 🟦	SOC feed outlet temperature 🟦
P (C2O)	Sweep heater outlet temperature setpoint* 🟧	SOC sweep outlet temperature 🟧



- Plantwide PI control setup with cascade control
- Compare to NMPC, which is better able to handle variable interactions and constraints

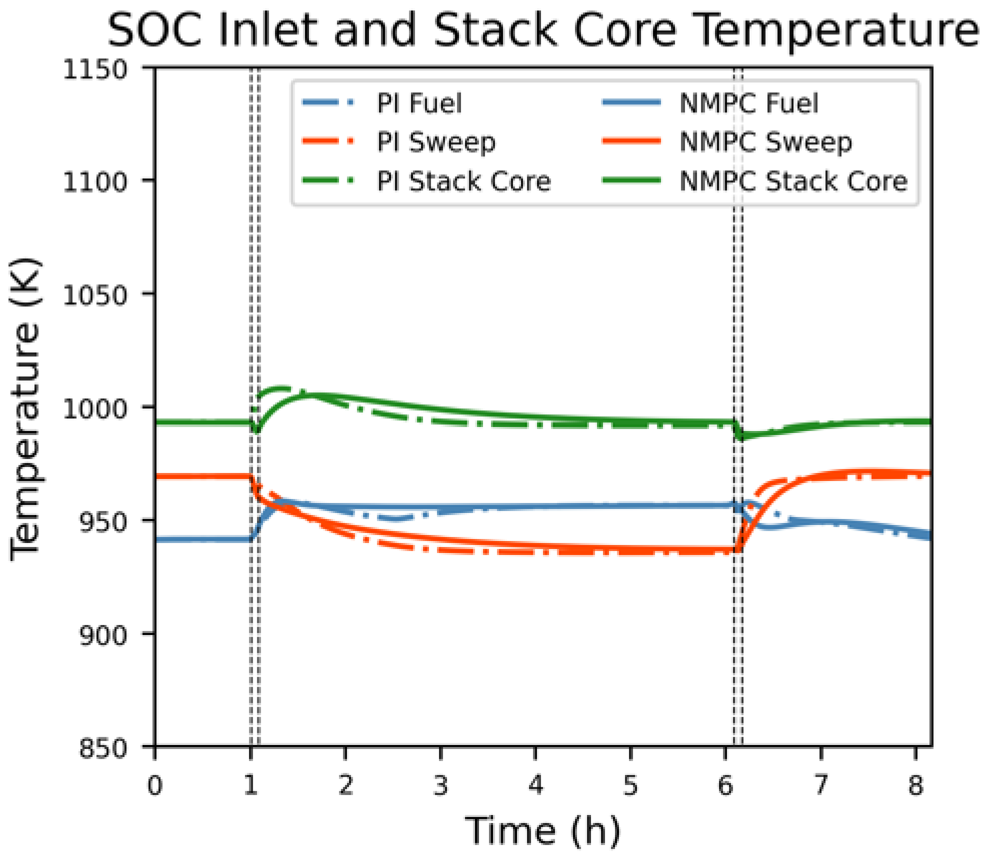
SOC-IES Case Study: Comparison of PI control to NMPC

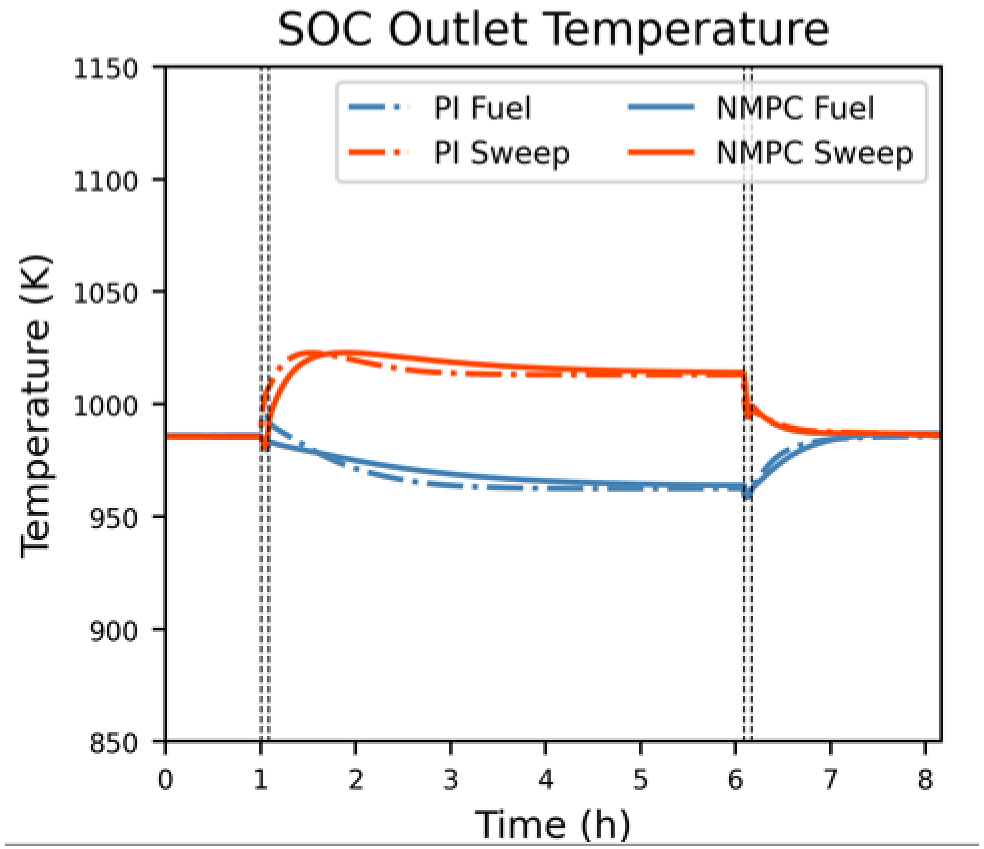
- Both PI and NMPC quickly transition between setpoints for maximum H_2 production to power generation (within 5-10 minutes) and back
- PI overshoots on power usage, whereas NMPC does not
  - Possibly able to be smoothed over by a local battery
- Both control methods are able to achieve a rapid transition



NMPC --- solid line
PI --- dashed line

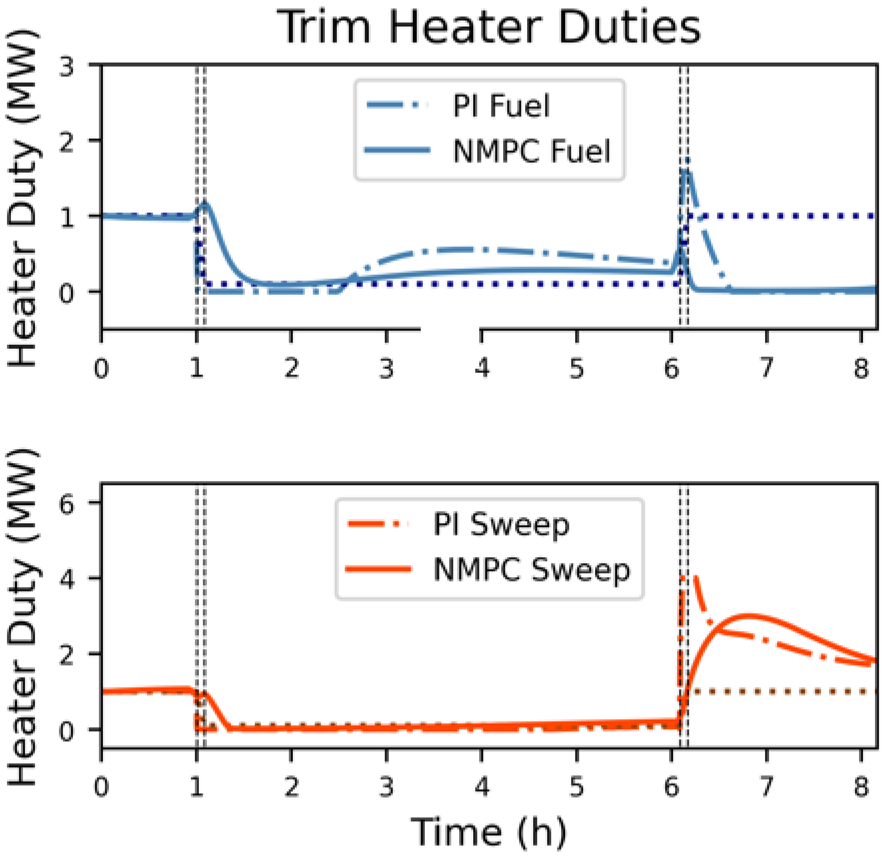
SOC-IES Case Study: Slow Thermal Dynamics

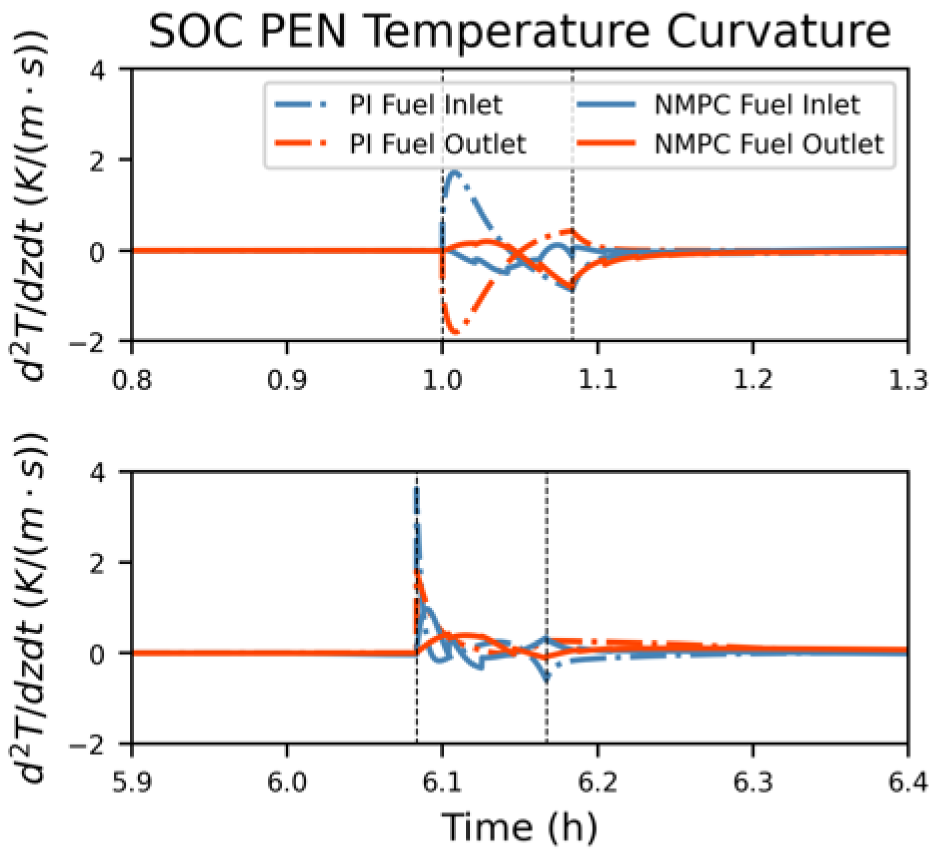

SOC Inlet and Stack Core Temperature


SOC Outlet Temperature

- H_2 production responds immediately, but temperature takes hours to settle

SOC-IES Case Study: Trim Heaters and Mixed Partials



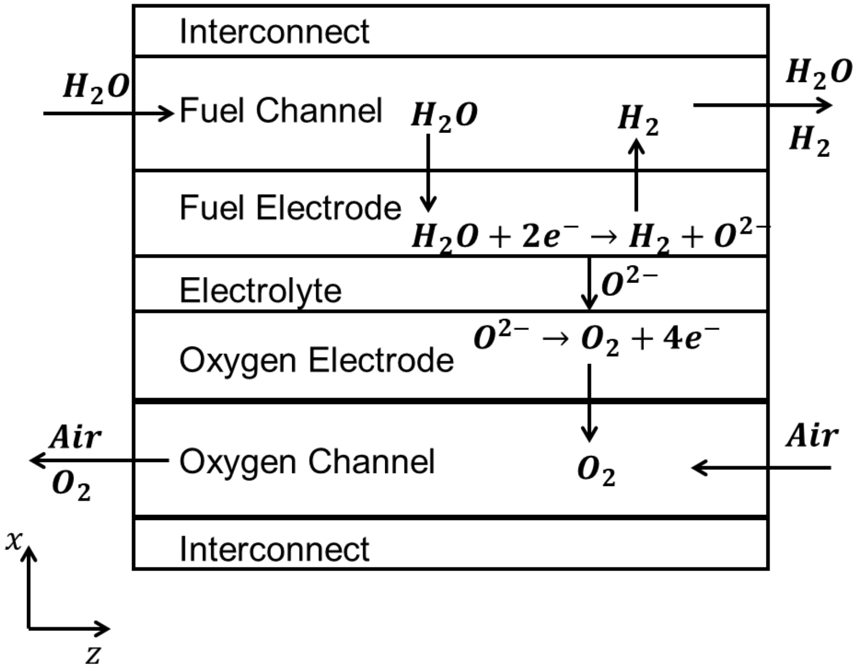


- Trim heaters are still engaged at end of time period, indicating the entire system is not at steady state yet
- NMPC can minimize magnitude of time derivative of cell temperature gradient (mixed partial) in order to reduce thermal failure probability

Case Study: SOEC Degradation Modeling

- Due to degradation, **SOC performance is time-varying**.
- Optimize SOC system performance over **cell's entire lifespan** to maximize net present value (NPV)
- Cell experiences both **physical** and **chemical degradation.**
- Due to mass and heat integration, it is desired that the entire SOC-IES be considered.
- Results presented are for **electrolysis mode only.**
- Long timescales (up to 20,000 hours) mean that **everything in IES besides cell is at steady-state**

SOC degradation work by Nishant Giridhar, Quang Minh Le, and Debangsu Bhattacharyya at WVU, more details on poster



Planar fuel electrode supported SOC

Materials
- Fuel electrode – Ni-YSZ
- Oxygen electrode – LSM-YSZ
- Electrolyte – YSZ

Modeling details
- First principles dynamic 2-D, non-isothermal equation-oriented model
- Capable of SOFC and SOEC operation
- This work - SOEC

SOEC Microstructure Degradation Modeling

- Degradation occurs over thousands of hours

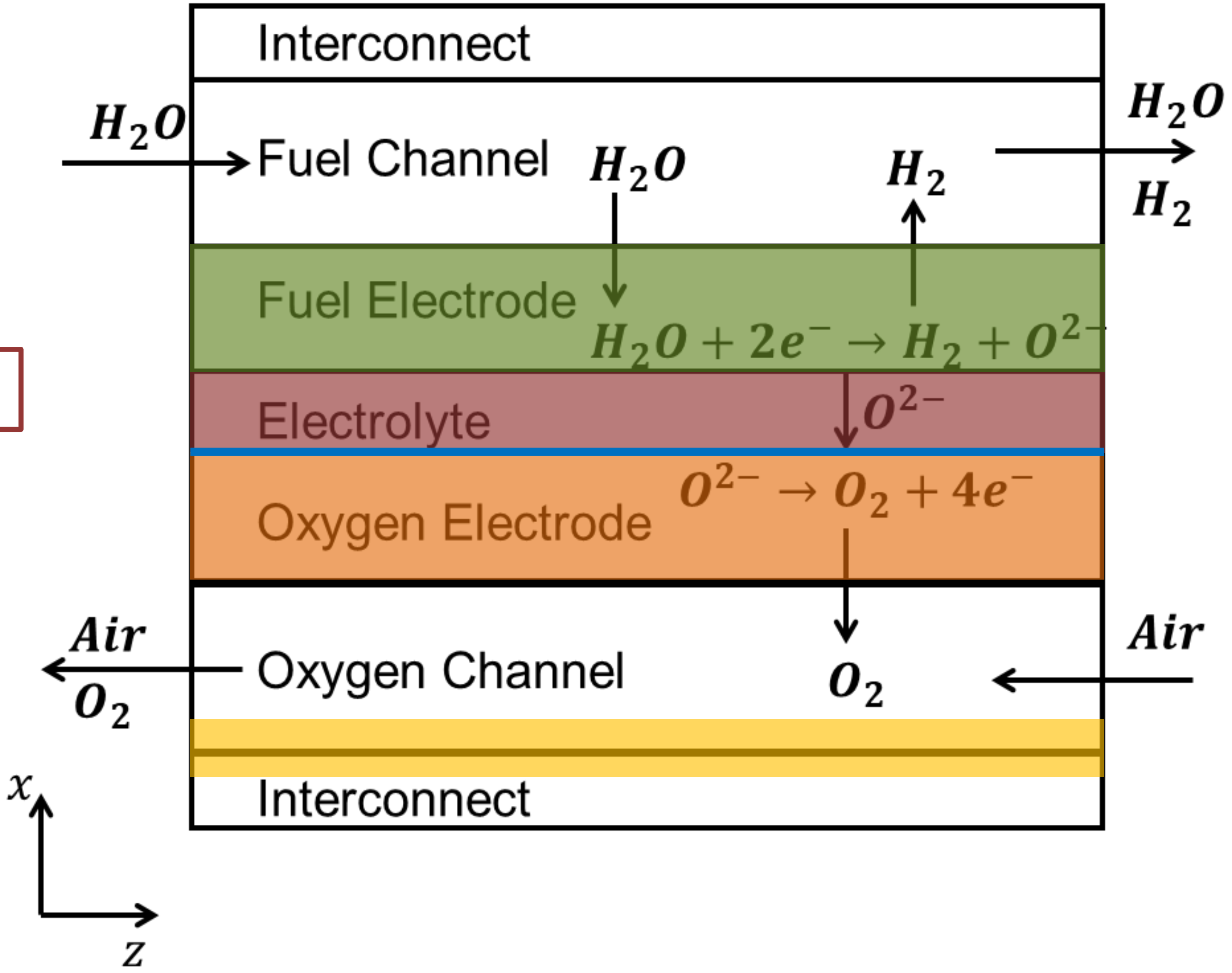
Fuel electrode Ni agglomeration

YSZ electrolyte phase transformation

LSM-YSZ phase coarsening

Lanthanum zirconate scale growth

Chromium oxide scale growth



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)

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

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

Target stack replacement costs

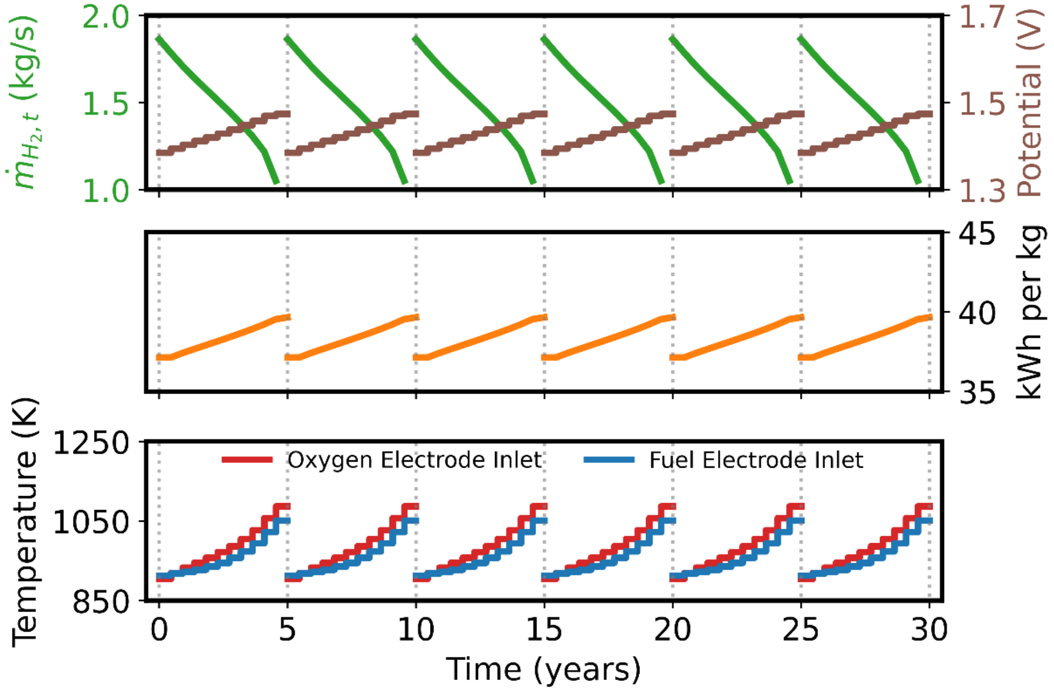
Decrease degradation through operating conditions

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

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

Selected Replacement Schedules in Two Markets

Electricity Cost = 0.03 \$/kWh

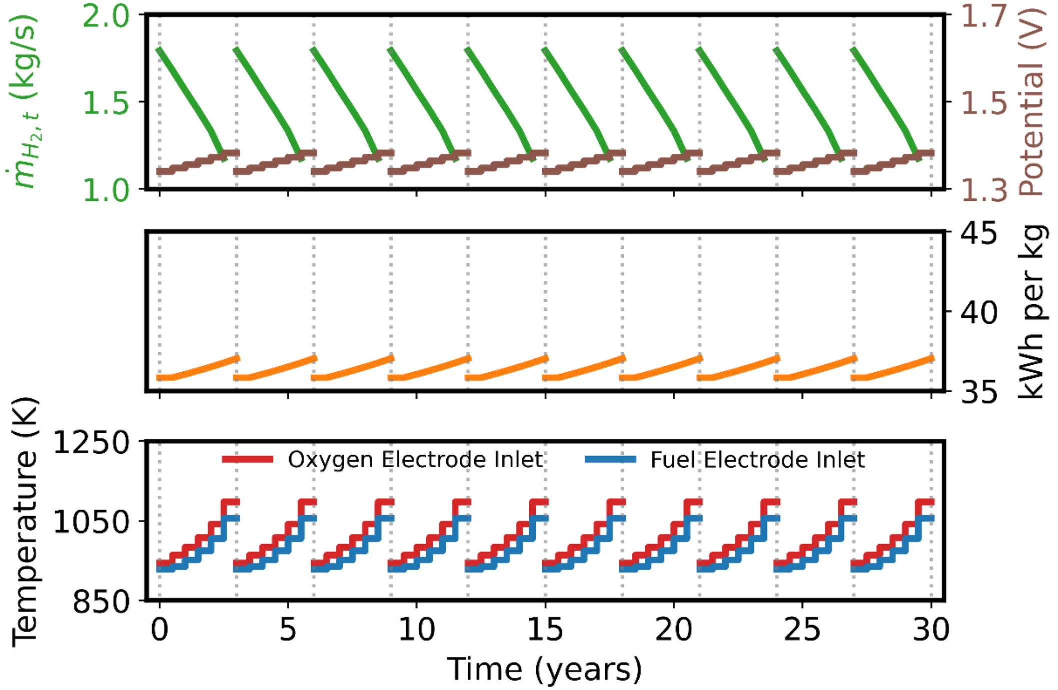


Replacement time = 5 years

Average Sp. Energy Consumption = $38.0\,\frac{kWh}{kg\ H_2}$

Average Degradation rate = 3% /khr

Electricity Cost = 0.3 \$/kWh



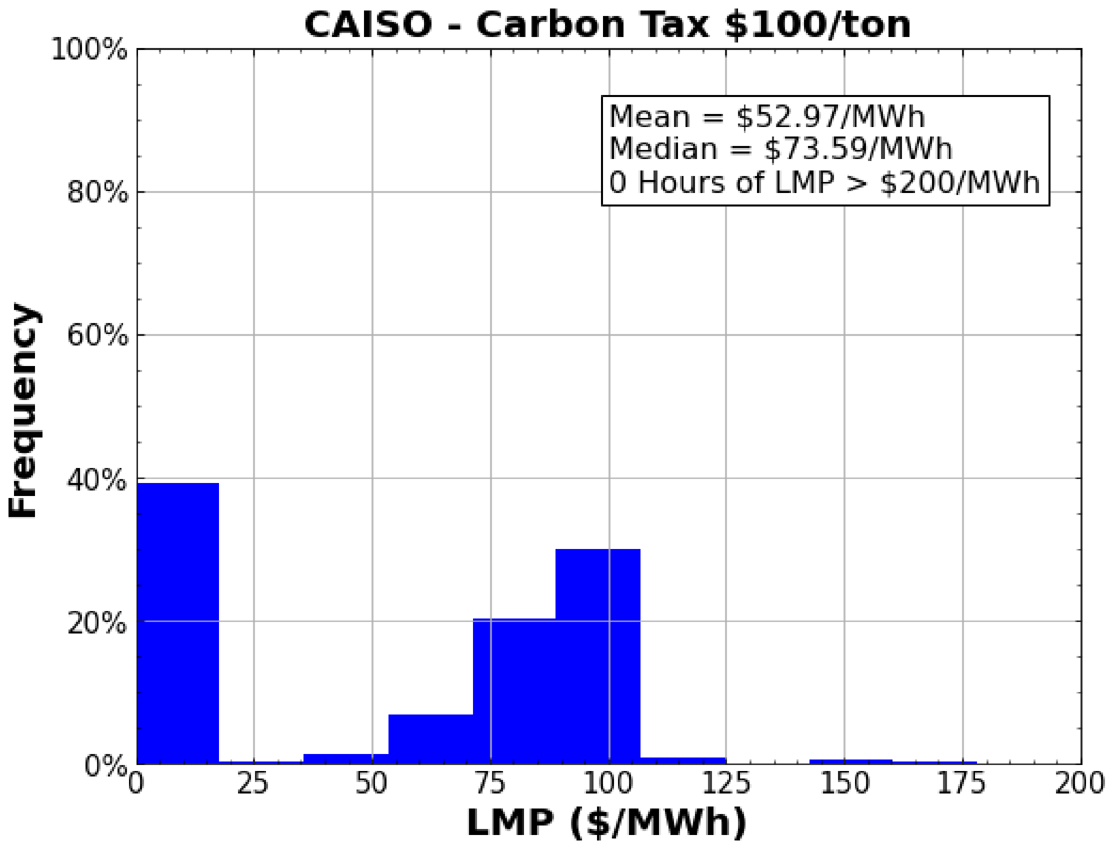
Replacement time = 3 years

Average Sp. Energy Consumption = $35.8\,\frac{kWh}{kg\ H_2}$

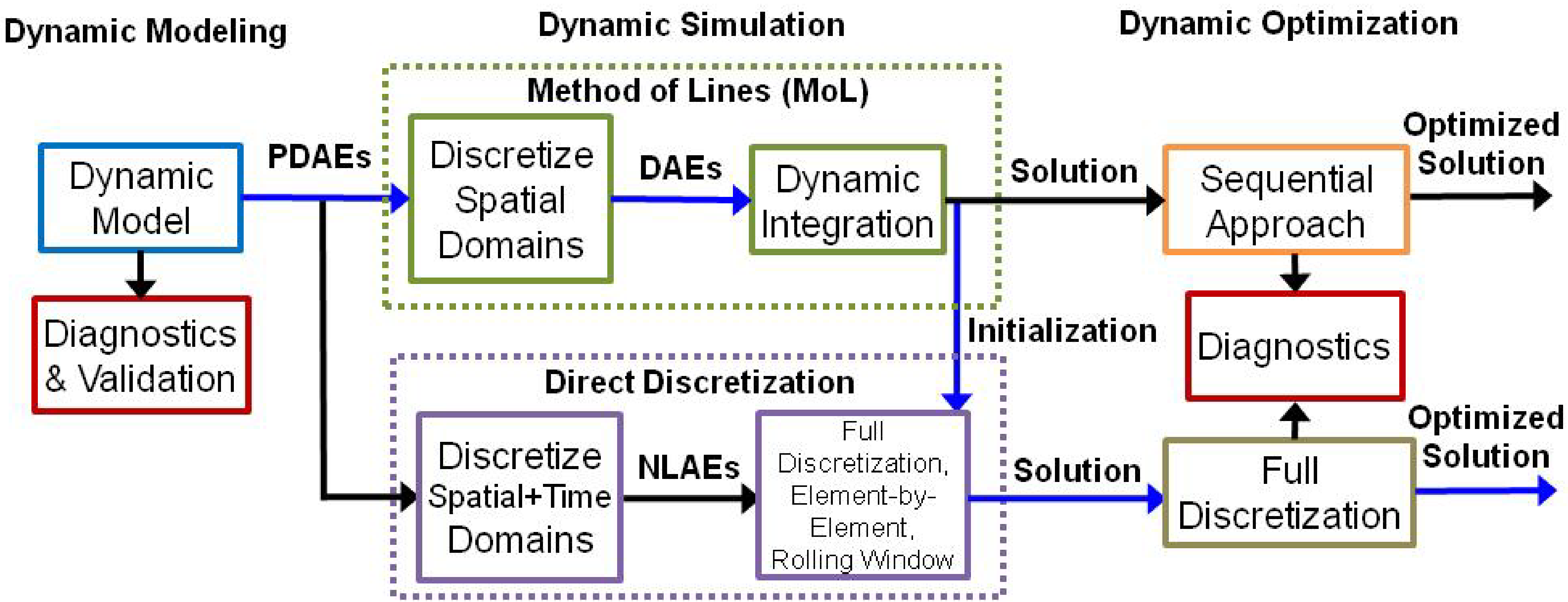
Average Degradation rate = 4% /khr

Conclusions

- Due to fluctuating demand and electricity prices, plants are rarely at steady state
- IDAES offers a framework to combine steady state modeling, multiperiod modeling, and full dynamic modeling
- Tools are available for both simulation (though PETSc-TS) and optimization (through Pyomo DAE)
- Dynamics can range in time from seconds to years



Dynamics Questions



Questions about Pyomo/IDAES dynamic capabilities?

Contributors to this research:

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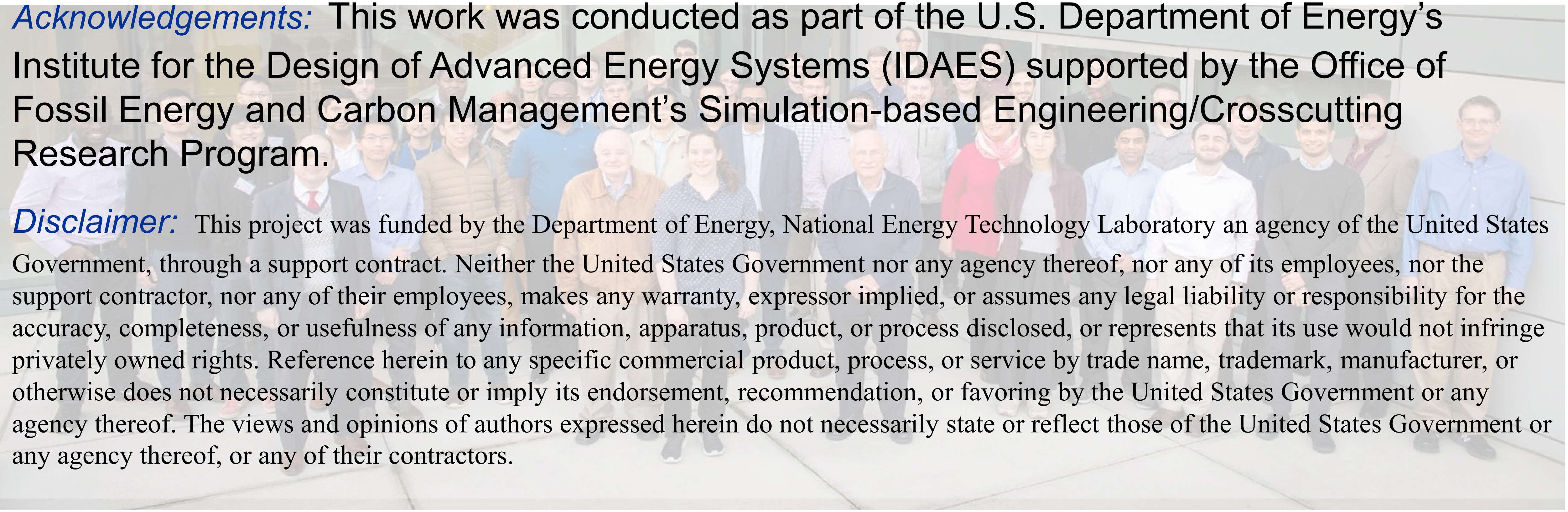
- **University of Notre Dame**: Alexander Dowling, Xian Gao



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