Evaluating Advanced Hybrid Energy Systems with IDAES

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10-11-2023

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IDAES Institute for the Design of Advanced Energy Systems

Design and Evaluation of Integrated Systems for Net Zero Emission

EMRE Collaboration

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EMRE Project Objective

- Develop an **optimization framework** to determine the best **process configuration** to achieve net-zero/net-negative emissions in NGCC power plants.

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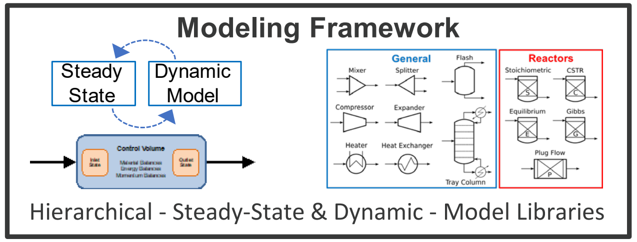
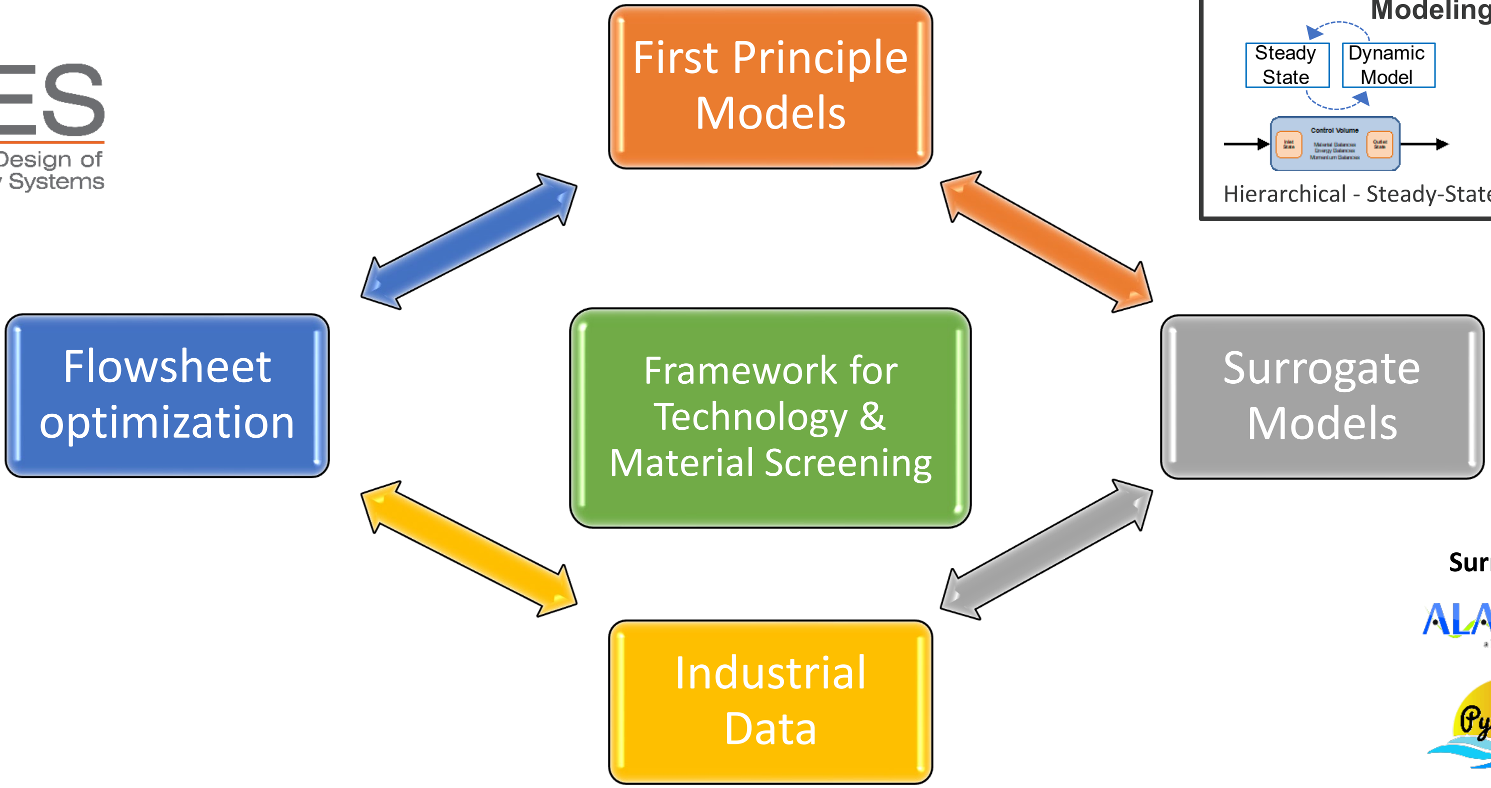
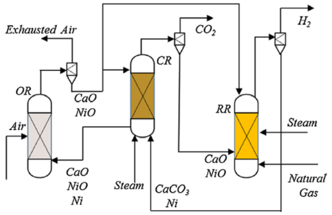




Plant Design Process Optimization



AI/ML Surrogate Modeling

ALAMO
a black-box modeling tool

PySMO

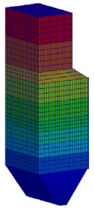
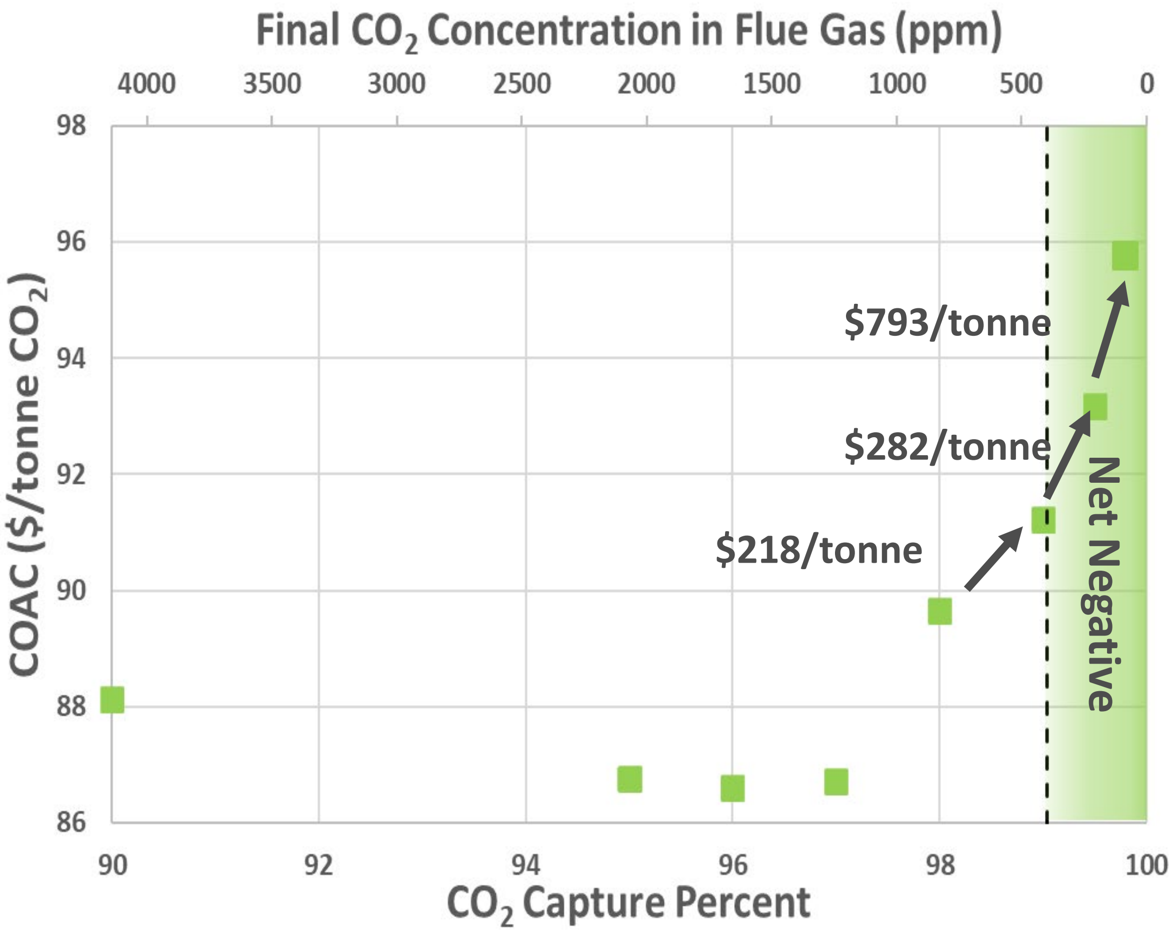


Figure 1. Technical approach

Motivation

- **Net zero emissions from low CO_2 concentrations:**
  - Energy intensive + expensive process + process operability
- **Integrated energy systems are critical for reaching net negative and net zero emissions.**
- **Identifying the level of integration is an open question.**
  - NGCC + PCC + polishing step or DAC
  - Power and heat from NGCC or electric boiler



Hybrid/Integrated Energy Systems

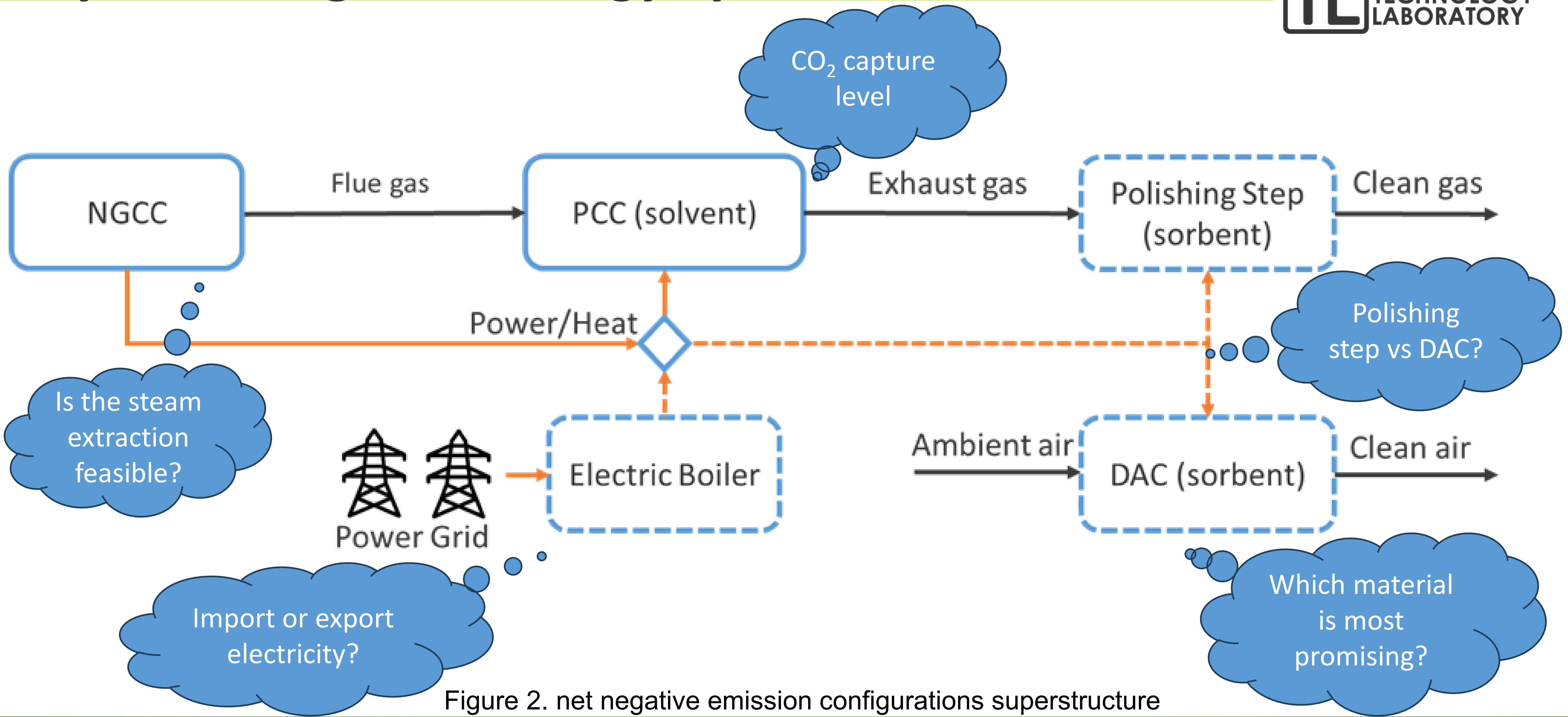


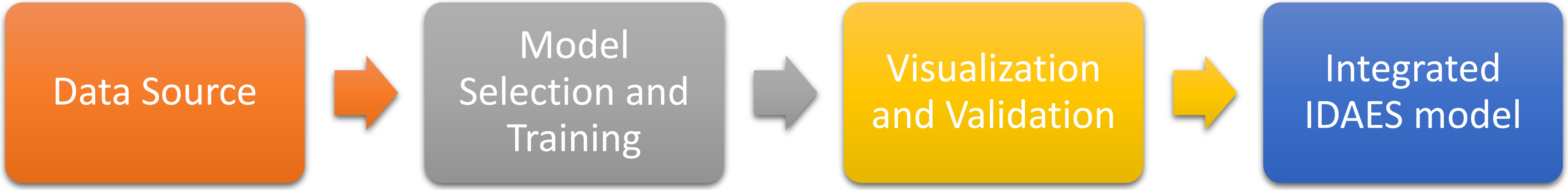
Figure 2. net negative emission configurations superstructure

Key Questions – Industrial Collaboration

- Can the addition of a polishing step or DAC system reduce the cost of achieving net-negative emissions compared to a standalone PCC?
- Which material achieves the lowest cost of capture?
- How do EMRE's materials compare to adsorbents found in the literature?
- How does a DAC system compare to the PCC + polishing step cases?

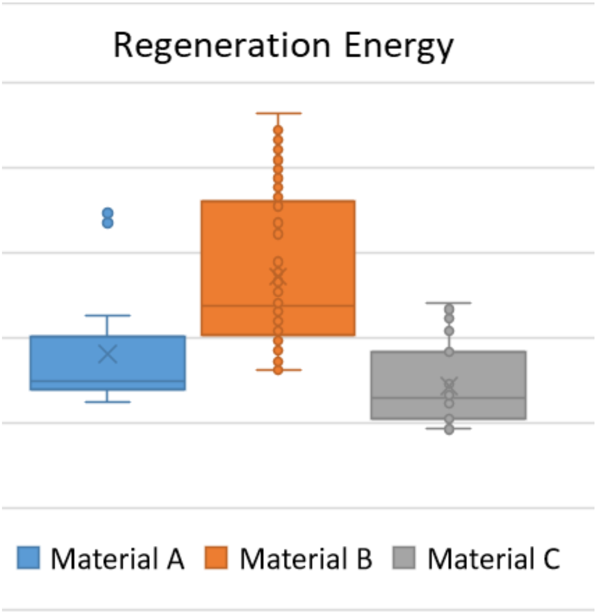
How to Leverage Legacy Models?

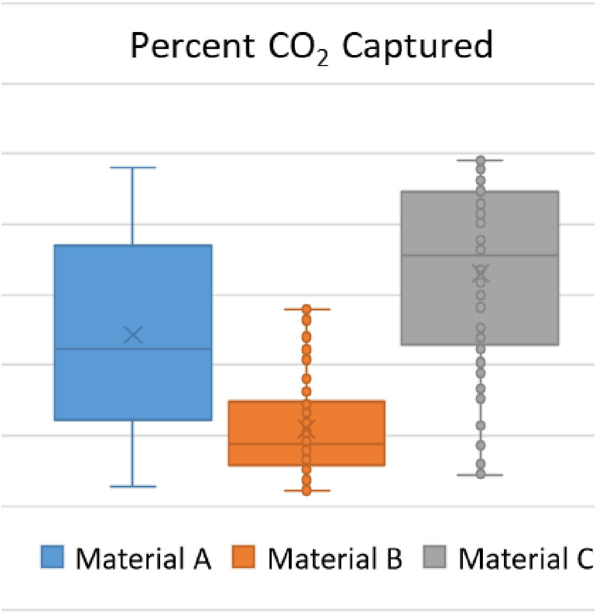
- **IDAES framework – workflow:**

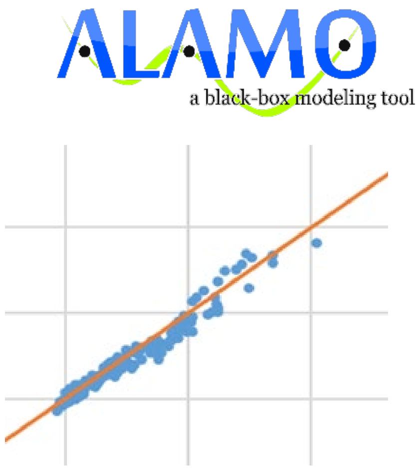


Inputs: air velocity, purge temperature and pressure, cooling temperature

Outputs: DAC system performance (regeneration energy and recovery)







Optimization Formulation

$$\min_{t_{ads}, T_{cool}, T_{purge}, v_{air}} \quad CO_2\ cost\left(\frac{\$}{Tonne}\right)$$

$$\boldsymbol{CO_2\ cost} = \frac{\boldsymbol{Annualized\ CAPEX + Fixed\ O\&M + Variable\ O\&M}}{\boldsymbol{CO_2\ Captured}}$$

$s.t.$

$Performance\ Surrogates$	$Detailed\ TSA\ model$
$tmin\ s \leq t_{ads} \leq tmax\ s$	$T_{ads} - T_{cool} \geq 10\ K$
$Tmin\ C \leq T_{cool} \leq Tmax\ C$	$T_{heat} - T_{des} \geq 10\ K$
$Tmin\ C \leq T_{purge} \leq Tmax\ C$	$T_{ads} \leq T_{des}$
$vmin\ \frac{m}{s} \leq v_{air} \leq vmax\ \frac{m}{s}$	$350\ K \leq T_{heat} \leq 500\ K$
	$3500\ Pa \leq \frac{\Delta P}{bed} \leq 4500\ Pa$

Operating Constraints

$+$

$$target\ \dot{n}_{CO_2} = PCC\ \dot{n}_{CO_2} - total\ DAC\ \dot{n}_{CO_2}$$

$$target\ \dot{n}_{CO_2} = 9.41\ mol/s$$

$$total\ DAC\ \dot{n}_{CO_2} = DAC\ unit\ \dot{n}_{CO_2} * n_{DAC\ units}$$

$$n_{DAC\ units} \geq 1$$

Desing constraints

$$n_{panels} = \frac{t_{ads}}{t_{cycle} - t_{ads}} + 1$$

$$\dot{m}_{air} \propto v_{air} * CSA_{brick} * n_{bricks} * n_{panels}$$

$$\dot{m}_{CO_2} \propto CO_2\ productivity * n_{bricks} * n_{panels}$$

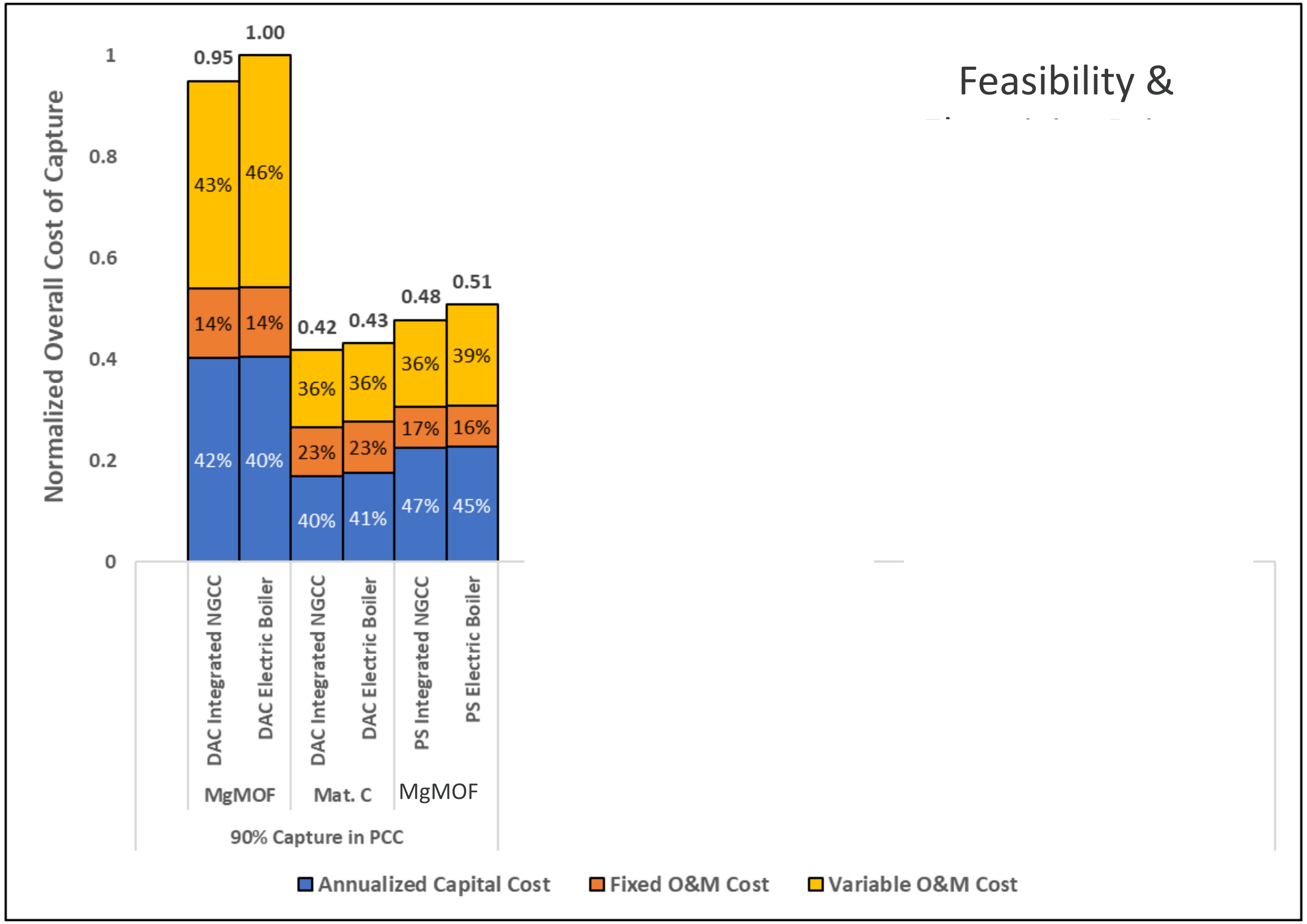
$$total\ regen\ duty \propto \dot{m}_{CO_2} * SRD$$

Costing model inputs

Integrated System to Achieve Net Zero Emissions

- 90% CO_2 capture + DAC not the best option
- Polishing step better than DAC
- 97% capture in PCC + polishing/DAC is the best option

Developed framework for material and technology screening for net-zero emissions



Poster: An Optimization Framework for Net Negative NGCC Power Plants – Alex Noring

IDAES Gas-Solid Contactor Models Used for Direct Air Capture

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Modeling Needs

Simplified Model → Equilibrium-based 0D shortcut model → Equilibrium-based 1D model → Rate-based 1D model

Simplified Model

- Separation fixed
- Pressure drop computed
- Cycle times assumed

Equilibrium-based 0D shortcut model

- Based on shortcut model proposed by Joss et al[1]
- Cyclical steady-state
- Adsorption is instantaneous
- Ideal gas
- No axial or radial gradients
- Assume cycle steps for adsorbent

Equilibrium-based 1D model

- Extend shortcut model to include axial variations in state variables
- Adsorption is instantaneous
- Ideal gas
- No radial gradients

Rate-based 1D model

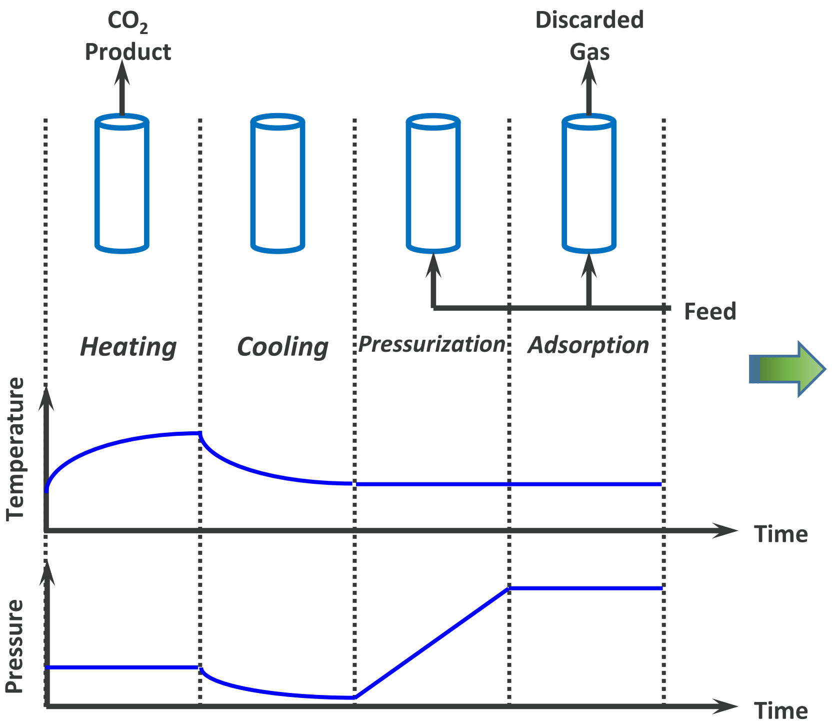
- Add rate equations
- Ideal gas
- No radial gradients

High Level Cost Estimation — **TEA – material performance and ambient conditions** — **Rigorous TEA**

1. *Joss L. Gazzani M, Hefti M, Marx D, Mazzotti M, "Temperature Swing Adsorption for the recovery of the Heavy Component: An Equilibrium-Based Shortcut Model", Industrial and Engineering Chemistry Research, 54,3027-3038, 2015*

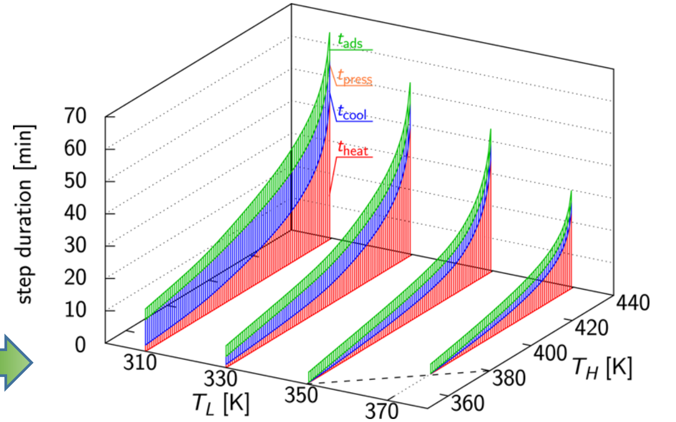
Modeling Needs: Custom 4 Step Adsorption Cycle

Overview of Equilibrium-based Shortcut Model

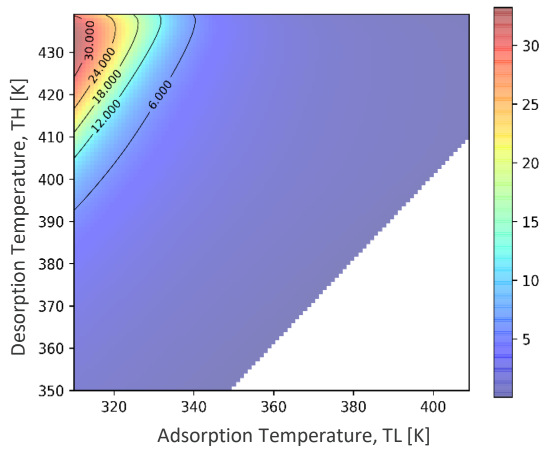


- **4 steps in a TSA cycle**
  - Heating step
  - Cooling step
  - Pressurization step
  - Adsorption step
- **Model Assumptions**
  - No axial or radial gradient in state variables
  - Ideal gas
  - External heating and cooling
  - Equilibrium between solid (adsorbed) and gas phases
    - Extremely fast mass transfer and adsorption/desorption rates

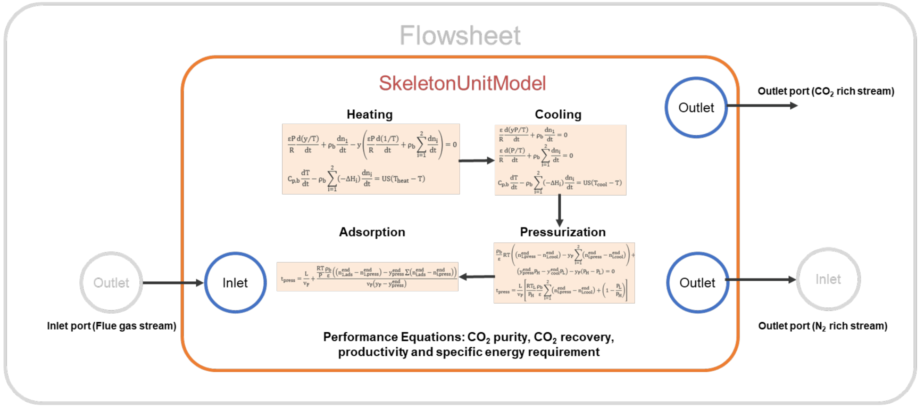
Effect of T_{ads} and T_{des} on Cycle Times



Productivity [kg CO2/(ton · h)]

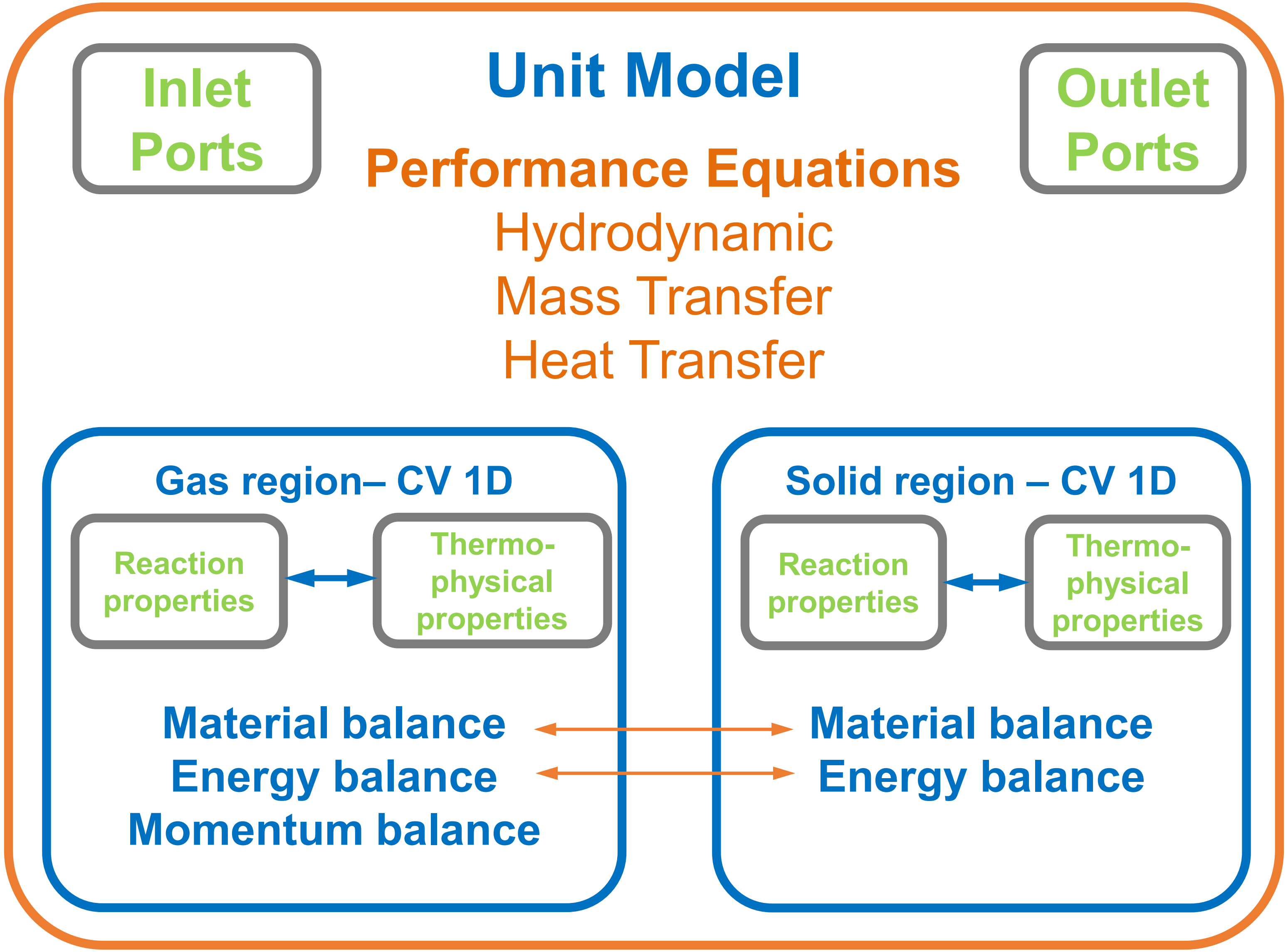


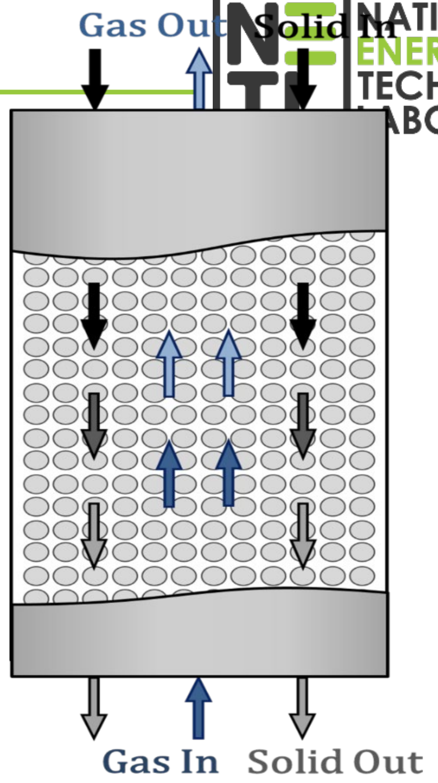
IDAES Implementation



1. Joss L. Gazzani M, Hefti M, Marx D, Mazzotti M, *"Temperature Swing Adsorption for the recovery of the Heavy Component: An Equilibrium-Based Shortcut Model", Industrial and Engineering Chemistry Research, 54,3027-3038, 2015*

Gas – Solid Contactor





Modifying hydrodynamics and momentum balances:

- Moving bed reactor
- Fixed bed reactor
- Bubbling fluidized bed reactor
- Rotatory packed bed reactor (pyomo)

Hybrid Energy Systems in IDAES
FLECCS and POWER to X

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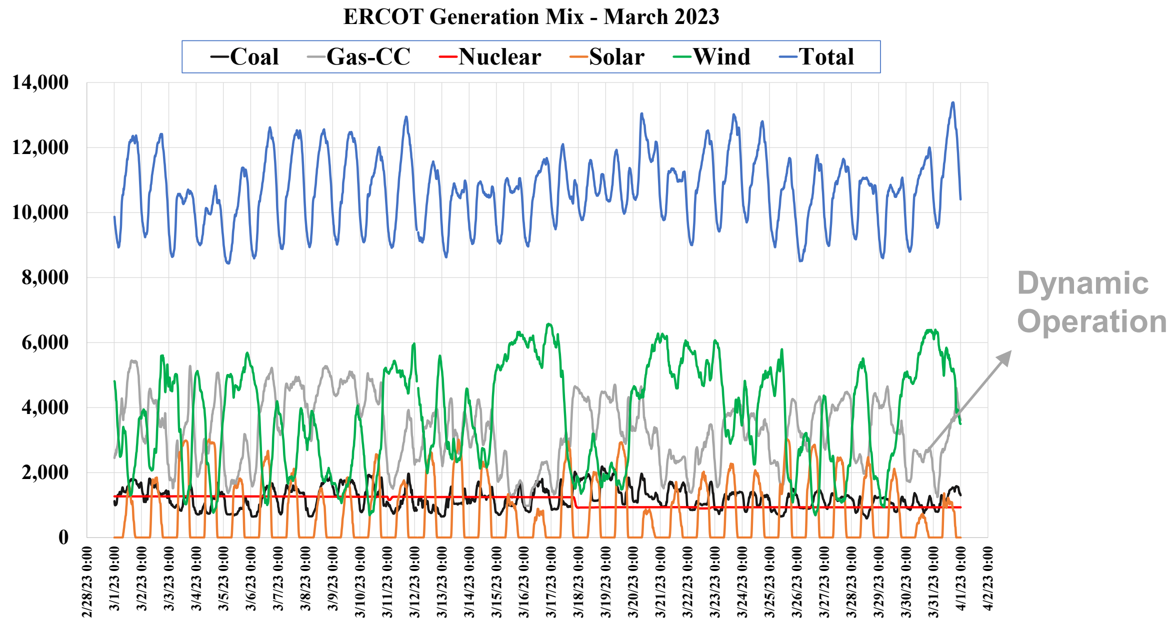
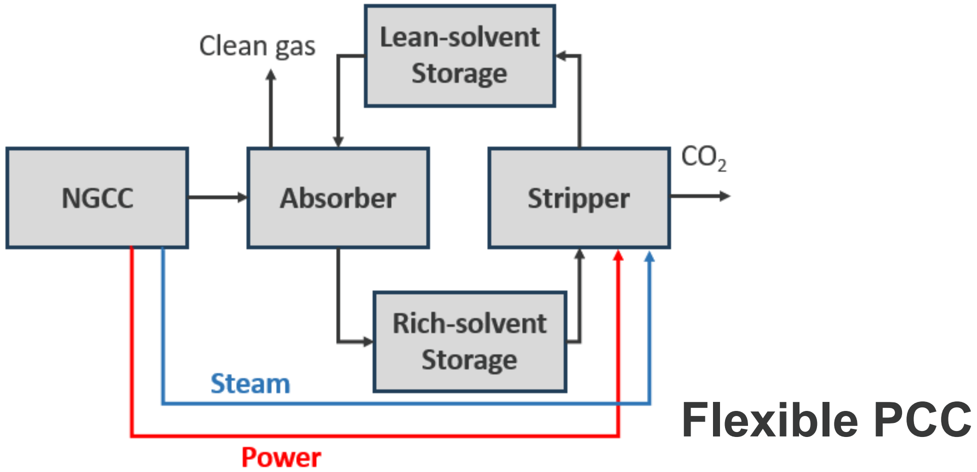
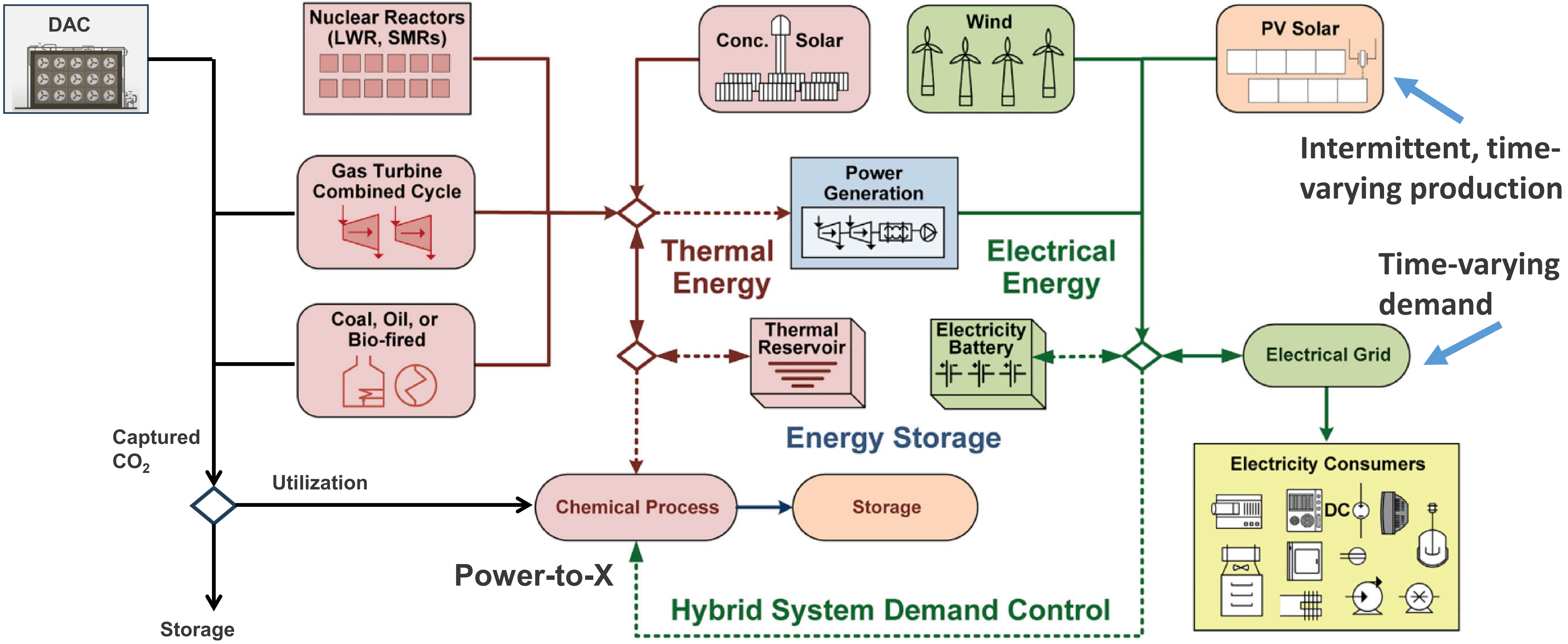
IDAES Grid Integration Tools for Flexible Systems

- Traditional TEA is more suitable for baseload operation
- Load-following operation is more realistic
- Flexibility is essential
  - Can PCC + Polishing step/DAC operate in a load-following manner?
- How to improve flexibility?
  - Load-shifting via solvent/sorbent storage – Regenerate solvent during off-peak hours
  - Load-shifting via DAC – Operate DAC at a higher capacity during off-peak hours
- For a given a time-varying load/prices, IDAES grid integration tools help
  - Determine optimal size of absorber, stripper, storage tanks, DAC system, etc.





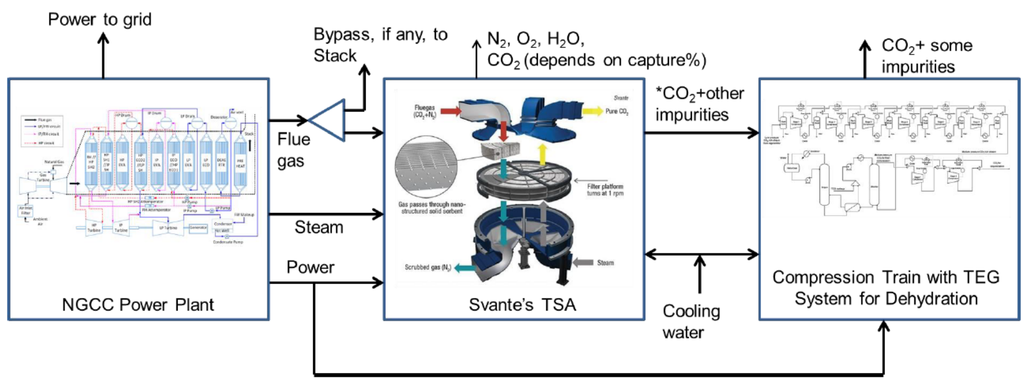
IDAES Enables Market-informed Analysis of HES



Arent et al. (2021) Multi-input, Multi-output Hybrid Energy Systems, Joule 5, 47-58.

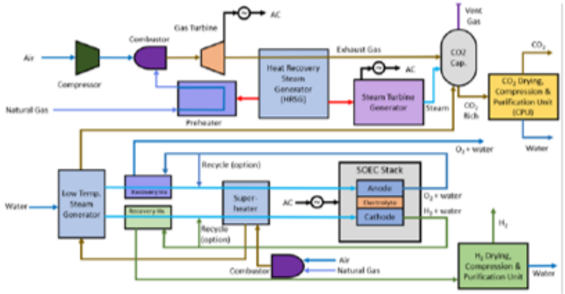
IDAES Market Analysis: Successful Case Studies

Develop Rigorous and Reduced-order (surrogate) Process Models

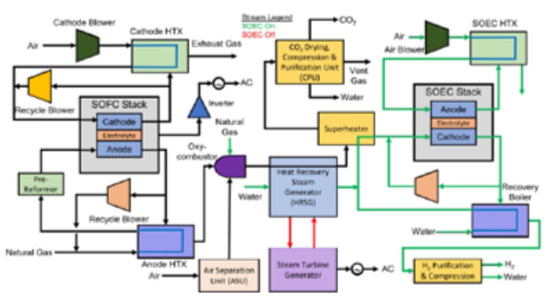


FLExible Carbon Capture and Storage (FLECCS)

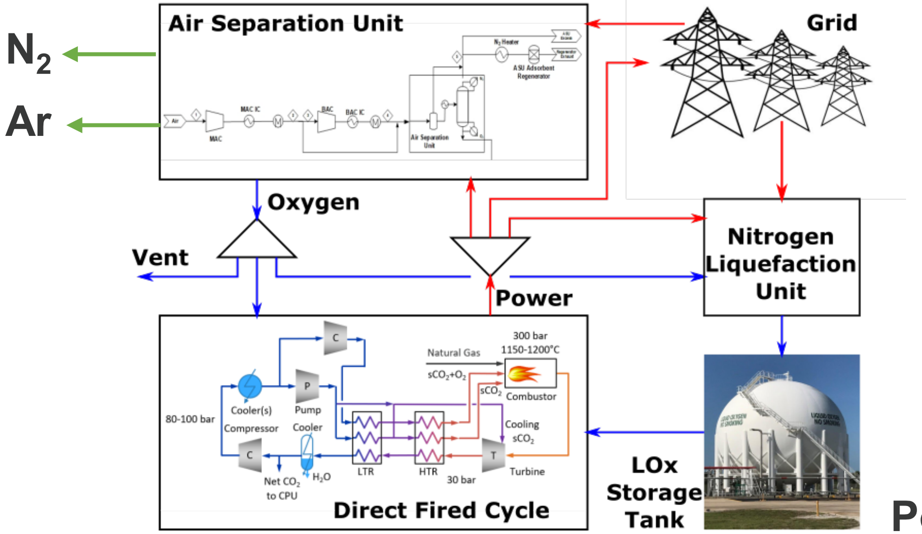
NGCC + SOEC
Power, Hydrogen, Coproduction



SOFC + SOEC
Power, Hydrogen, Coproduction



Power-to-H2: SOFC/SOEC Integrated Energy Systems

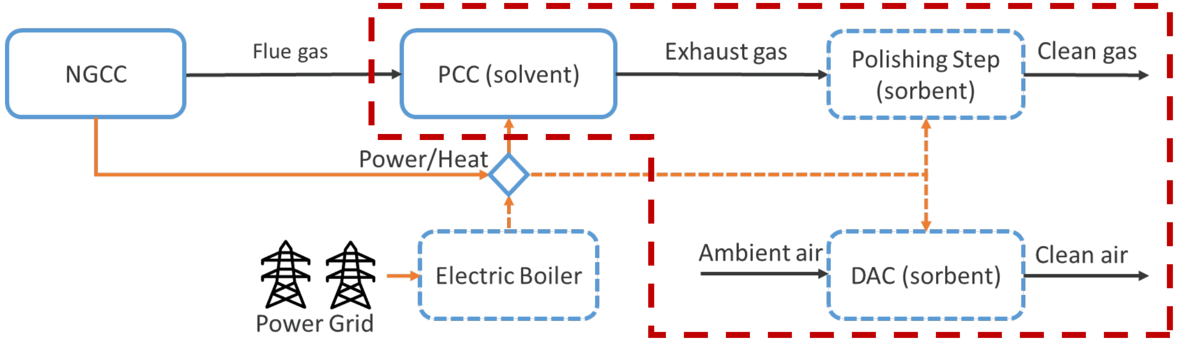


Power-to-argon/nitrogen: Allam-Fetvedt Cycle

Additional Slides

Optimization Formulation - Phase III

Proposed optimization framework to achieve net-zero emissions for NGCC power plant



Scope of Phase III Optimization

$$\min_{u_{DAC},\, u_{PCC},\, d_{PCC}} \quad Total\ CO_2\ cost \left(\frac{\$}{Tonne}\right)$$

$$\begin{aligned} s.t. \quad & DAC\ Performance\ Surrogates \\ & DAC + PCC\ Costing\ Model \\ & Net\ Negative\ Emission\ Constraints \\ & \boldsymbol{Detailed\ PCC\ Model} \end{aligned}$$

Phase III Optimization

- PCC design and operating variables included in optimization
- Determine the optimal capture rate (PCC)
- Minimize cost of capture (PCC + polishing step)

Project Timeline – Accomplishments

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- Established a CRADA agreement NETL – EMRE - 6 months
- Developed first round of flowsheets, models, property packages –
- Delivered first round of recommendations – year 1
- Delivered report with

Team

- **NETL**
  - Miguel Zamarripa
  - Daison Caballero
  - Alexander Noring
  - Josh Morgan
  - Anca Ostace
  - Douglas Allan
  - Tony Burgard
  - Jaffer Ghouse

- **EMRE**
  - Justin Federici
  - Rodrigo Blanco
  - + Others

Questions/Comments

Summary of Work in 2022

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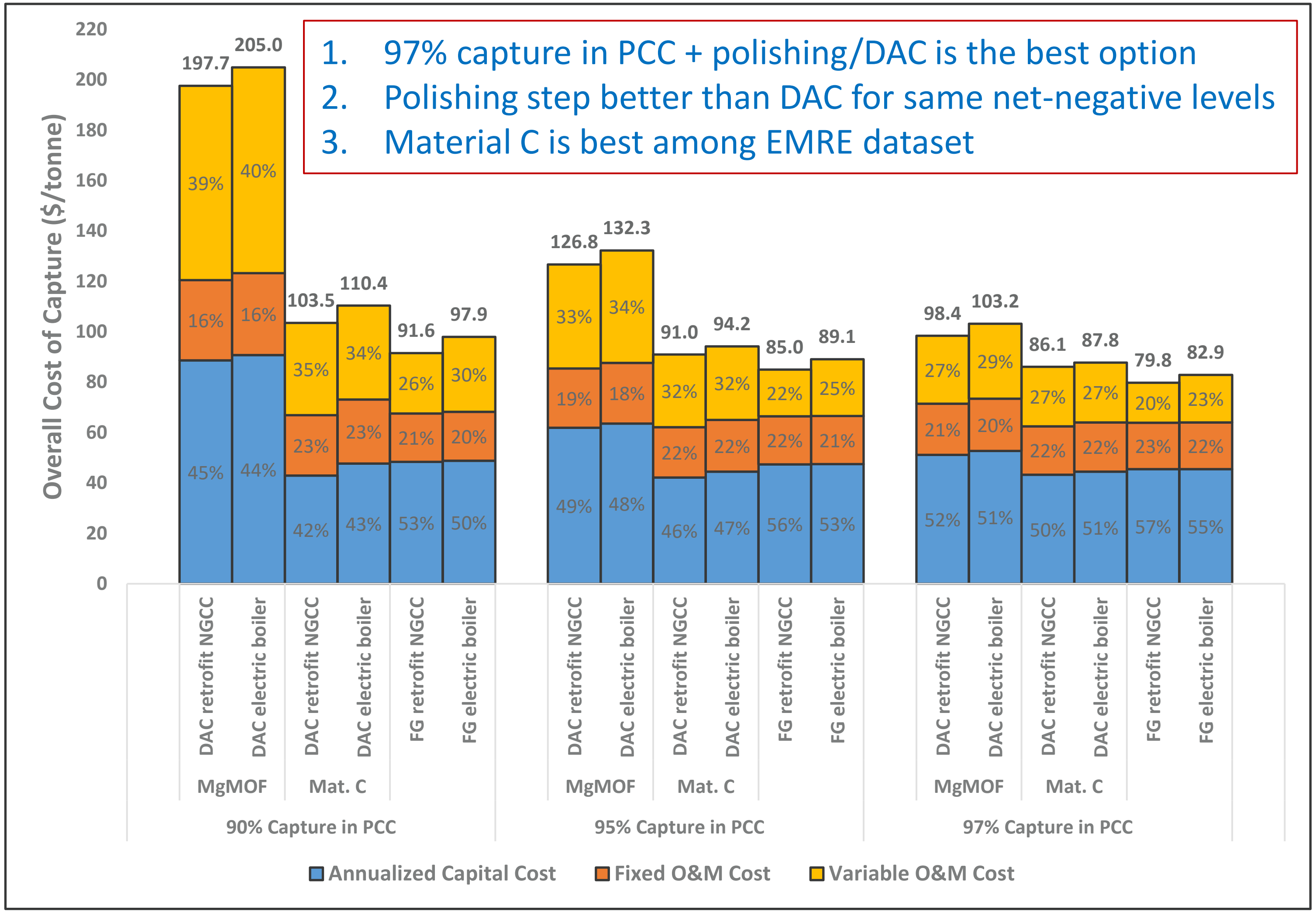
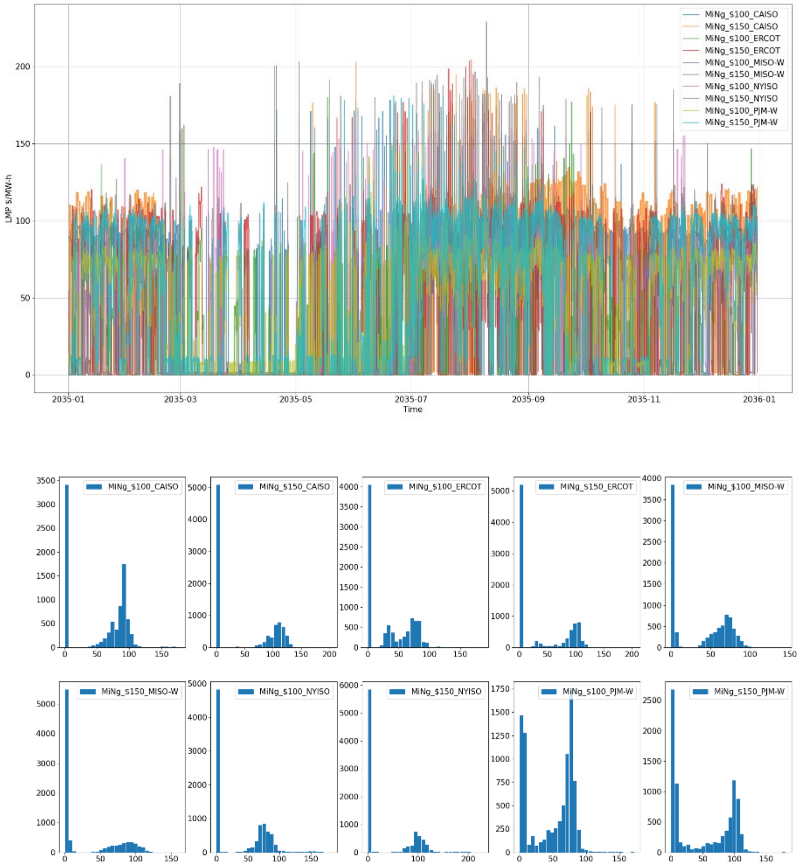
- **Improved costing estimates**
- **0D Equilibrium Model**
  - FG polishing step – Integrated NGCC & e-boiler (90%, 95%, and 97%)
  - DAC – Integrated NGCC & e-boiler (90%, 95%, and 97%)
- **EMRE DAC system data**
  - Link costing to data provided
    - — E-boiler case
    - — Integrated NGCC case
  - Costing estimate analysis for data
  - Performance surrogates for data
  - Use surrogates and costing in optimization
    - — DAC – Integrated & e-boiler case (90%, 95%, and 97%)
    - — Sensitivity on brick cost, replacement time, etc.



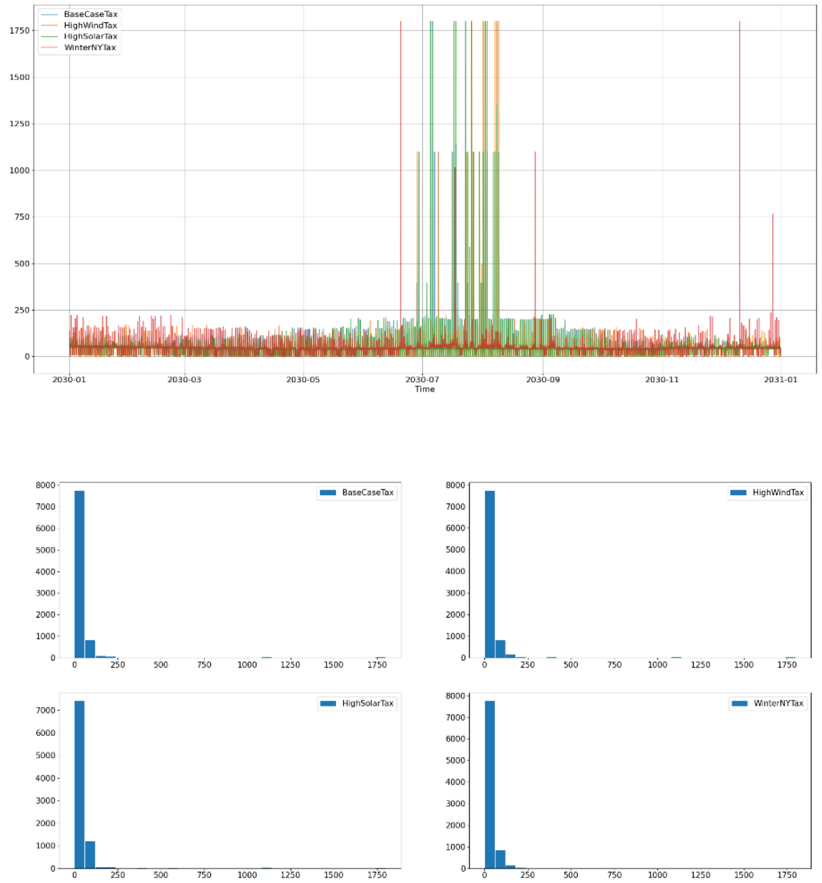
Incorporating Electricity Market Prices for Design

Problem: Given a high VRE grid in 2035 under different scenarios, will NGCC with flexible capture systems be economically viable?

Data Set 1



Data Set 2



Should capture system+DAC be built? (i.e., Is it cheaper to pay a carbon tax?)

If yes, what is the optimal size and capture rate?

How do various potential market scenarios impact results?

Multi-Period Stochastic Optimization Problem

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$$\max_{d,u_{t,s}} \overline{NPV} = \sum_{s \in S} p_s NPV_s = \sum_{s \in S} p_s \left(\sum_{t=1}^{n} \frac{Profit_{t,s}}{(1+r)^t} \right) - Capex_s$$

- Weighted average NPV across scenarios ($\overline{NPV}$)
- Weight associated with scenario s (p_s)
- Design/Capacity (d)
- Operating decisions ($u_{t,s}$)
- Set of scenarios ($s \in S$)
- Time set within scenario *s* ($t=1 \dots n$)

$$NetProfit(d,u_t) = (1-TAX)\Big[\overbrace{Revenue(d,u_t)} - \overbrace{Opex(d,u_t)} - CO_2\,Penalty(d,u_t) - \underbrace{FOM(d)} - \underbrace{VOM(u_t)} \Big] + TAX \times \underbrace{Depreciation(d)}$$

Revenue:
+ NGCC gross power
– Auxiliary power load
– Pump/blower work for TSA
– Power equivalent of steam
– Compression work

Opex:
+ Natural gas
+ Cooling water

FOM:
+ Power plant(LADWP)
+ TSA unit
+ Compression train
+ Adsorbent replacement

VOM:
+ Minimum maintenance adder for power plant

Depreciation: Straight line depreciation with zero salvage value.

Incorporate TEA into optimization

Process Model Equations: $g(d,u_t,x_t) = 0, t \in T$

Operating constraints: $h(d,u_t,x_t) \le 0, t \in T$

$y_t \in [0,1]$ → Startup/Shutdown

$y_d \in [0,1]$ → Build/Not-build technology

- **Solve model for full year signal or representative days**
- **Solve for deterministic or stochastic problem**