IDAES

Institute for the Design of Advanced Energy Systems

A New Platform for Process Design & Optimization

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National Energy Technology Laboratory

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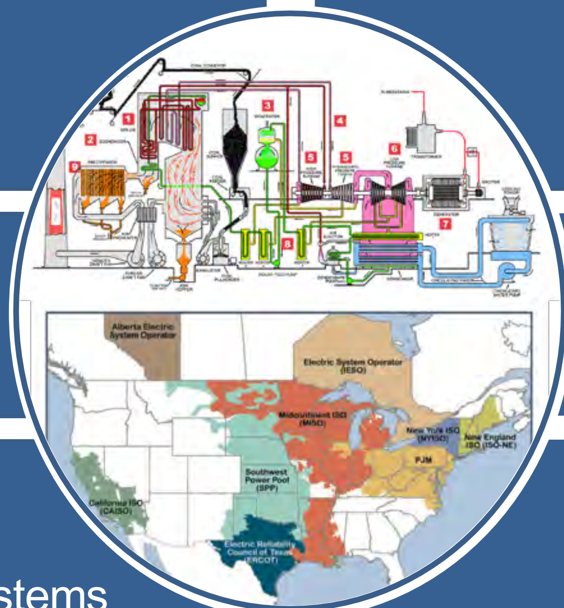
Increasingly dynamic operations

Greater linkages among scales

Support for innovative concepts, systems, and technologies:
Process Intensification; Hybrid Systems



30+ years of progress in algorithms, hardware, modeling approaches

Advances in continuous nonlinear optimization (dynamics, uncertainty)

Advances in discrete optimization (algorithms and formulation)

DOE Office of Fossil Energy Simulation-Based Engineering/Crosscutting R&D Program

Process Optimization: Transition to EO (algebraic) models

Optimization over degrees of freedom only

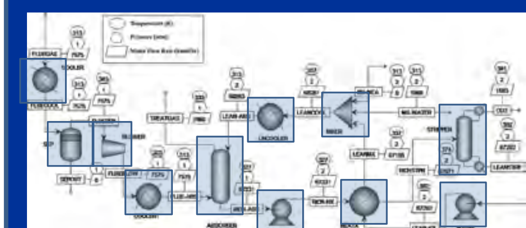
$$\min_{u} \quad f(u)$$

$$u^L \leq u \leq u^U$$

u

f

Simulator



Black-box optimization (DFO)
~ 100-1000 simulations

Glass-box optimization
~ 1-5 STE

Optimization with embedded algebraic model as constraints

$$\min_{x,u} \quad f(x,u)$$

$$h(x,u)=0$$

$$x^L \leq x \leq x^U$$

$$u^L \leq u \leq u^U$$

[Adapted from Biegler, 2017]

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Equation-Oriented (algebraic) models: Benefits

$$h(x,u)=0$$

$$\min_{x,u} \; f(x,u)$$
$$h(x,u)=0$$
$$x^L \leq x \leq x^U$$
$$u^L \leq u \leq u^U$$

- Explicit equations exposed to general numerical solvers and analysis tools
- Significantly faster computational performance: automatic differentiation, exposed structure
  - Fully integrated complex facilities (enterprise-wide)
  - DAE and uncertainty can be addressed in this form
- Separation of model from solver
  - Supports a wide range of Newton-based solvers
  - Same model used for different analyses (simulation, optimization, sensitivity, UQ)
- Automatic model transformation and reformulation (e.g., MPEC, GDP, DAE, Stochastic Programming)
- MINLP / global optimization with explicit expressions

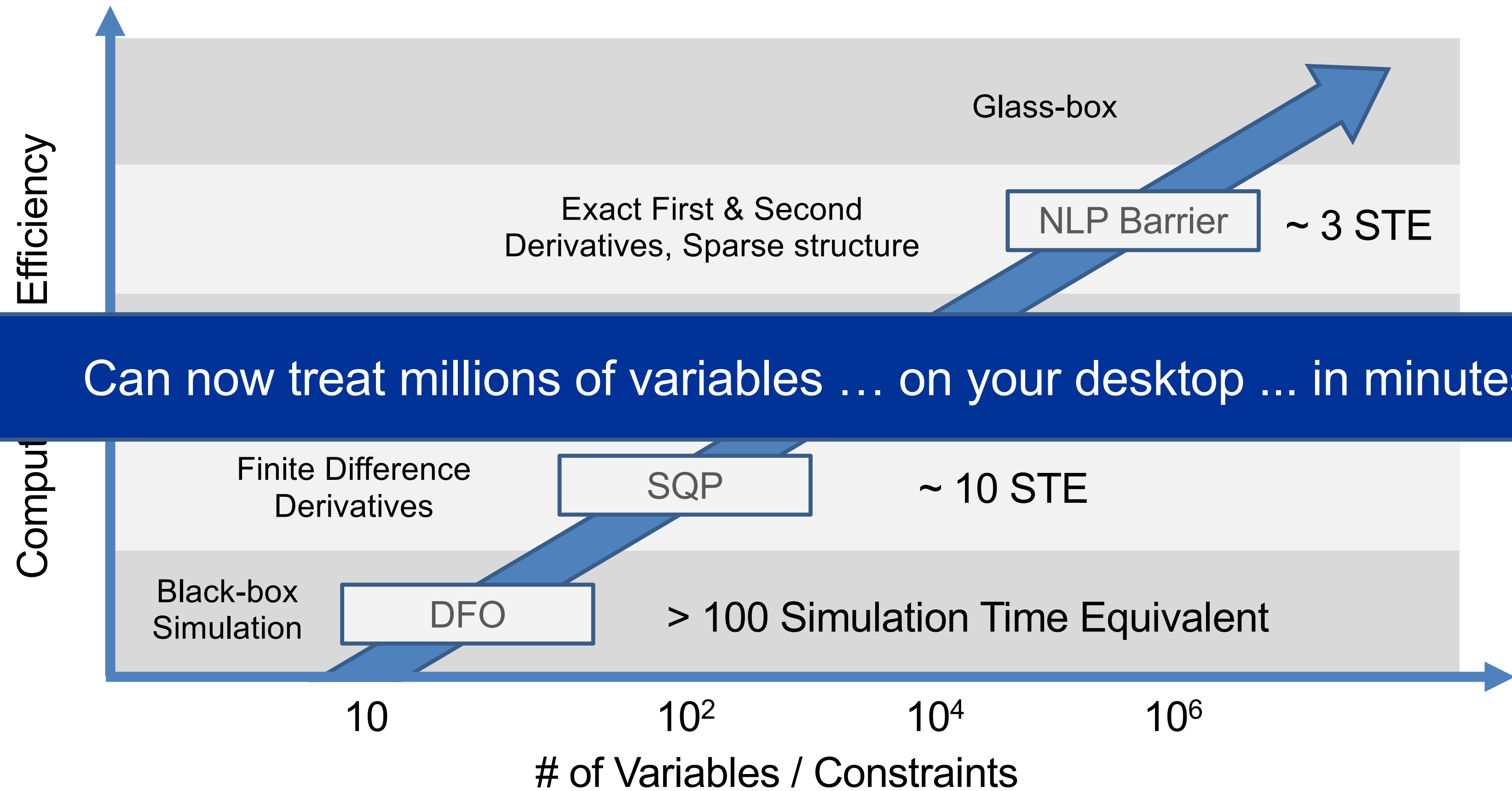
Equation-Oriented (algebraic) models: Challenges

$$h(x,u)=0$$

$$\min_{x,u} \; f(x,u)$$
$$h(x,u)=0$$
$$x^L \leq x \leq x^U$$
$$u^L \leq u \leq u^U$$

- Effective initialization critical for reliable convergence
- Not everything can (easily) be made equation-oriented
  - Need a strategy for black-box sub-components
- Nonlinear simulation and optimization formulations are much larger than black-box counterparts

Process Optimization Environments and NLP Solvers



[Adapted from Biegler, 2017]

Capabilities Needed for Design of Novel Energy Systems

Existing process unit model library for rapid assembly and modeling of flowsheets

Flexible capabilities to model novel technologies and optimize new materials

Efficient optimization tools to explore large space of potential process flowsheets

Construction of optimization-ready surrogates and physical property relations

Scalable identification and handling of uncertainty inherent in novel design

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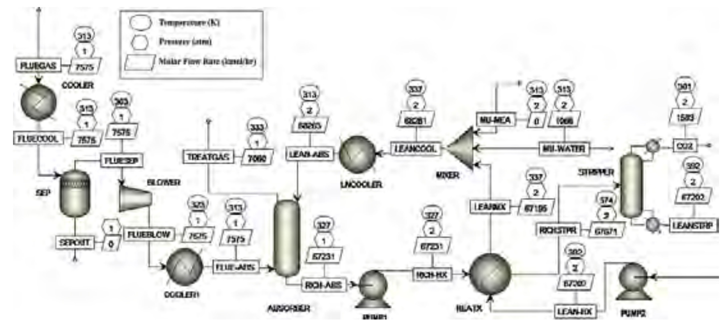
Sequential Modular Flowsheeting Tools

- Very capable for steady-state modeling of existing processes and techno-economic analysis



- Simulation-based, black-box analysis does not support “glass-box” optimization-based approaches
- Insufficient flexibility for easy creation of tailored models from existing sub-components
- Difficult to explore large space of potential flowsheets, typically focus on a few (design rules and experience)

Strong process modeling libraries – missing full “glass-box” for advanced optimization

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Image from: Kundu, Prodip & Chakma, Amit & Feng, Xianshe. (2014). Effectiveness of membranes and hybrid membrane processes in comparison with absorption using amines for post-combustion CO2 capture. International Journal of Greenhouse Gas Control. 28. 248–256.

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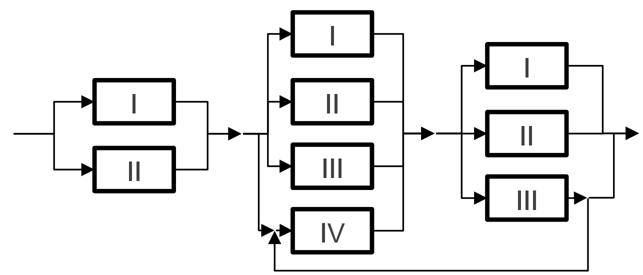
General Algebraic Modeling Tools (e.g., GAMS, AMPL)

- Superstructure optimization (reformulated as MINLP) well-supported by algebraic modeling tools (e.g., AMPL, GAMS)



- Algebraic modeling tools lack component-based, process engineering model libraries
- Significant expertise required to formulate the (manual) transformation to MINLP
- No capabilities for developing advanced algorithms

Strong “glass-box” capabilities – missing model libraries and extensibility for advanced algorithms

Capabilities Needed for Design of Novel Energy Systems

Capability needed	Next Generation Integrated Platform for Modeling and Optimization
Existing process unit model library for rapid assembly and modeling of flowsheets	IDAES Steady-state and dynamic equation-oriented model library and modular structure
Flexible capabilities to model novel technologies and optimize new materials	IDAES Steady-state and dynamic equation-oriented modeling framework
Efficient optimization tools to explore large space of potential process flowsheets	IDAES PyoSyn framework for superstructure optimization with Pyomo.GDP and GDPOpt
Construction of optimization-ready surrogates and physical property relations	ALAMO, HELMET, RIPE, PySMO: Optimization-based AI/ML approaches for kinetics, surrogate models, and thermo-physical properties
Scalable identification and handling of uncertainty inherent in novel design	Stochastic prog. & adaptive robust optimization for scalable, rigorous treatment of uncertainty

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Next Generation Integrated Platform for Modeling and Optimization

IDAES Integrated Platform

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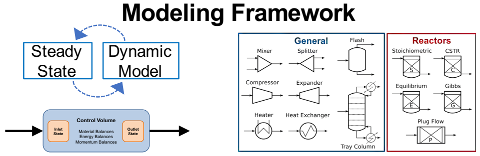
IDAES-Core

Modeling Framework



Hierarchical - Steady-State & Dynamic - Model Libraries

Data Management Framework

User Interface & Visualization

Advanced Equation Oriented Solvers

PYOMO

Flexible Programming Foundation

python

IDAES-Materials

MatOpt

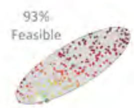
Nanomaterials optimization

IDAES-UQ

Data Reconciliation

K-Aug & sIPOPT

PyROS



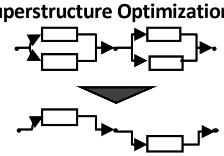
Parameter Estimation

Rigorous Model Sensitivity

Optimization & Uncertainty Quantification

IDAES-Design

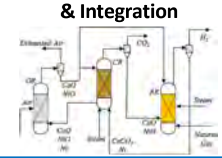
Conceptual Design via Superstructure Optimization



PYOMO GDP

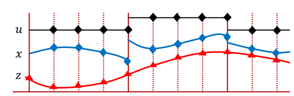
Pyosyn

Process Design, Optimization & Integration



IDAES-Operations

Process Dynamics



PYOMO DAE

Trajectory optimization, optimal control, state/parameter estimation

Process Control

caprese

IDAES-AI

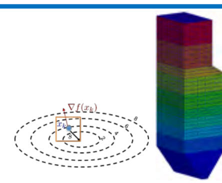
HELMET

ALAMO

a black-box modeling tool

RIPE

PySMO



Multi-Scale Modeling and Optimization

IDAES-Enterprise

Electricity Grid Modeling

Expansion Planning

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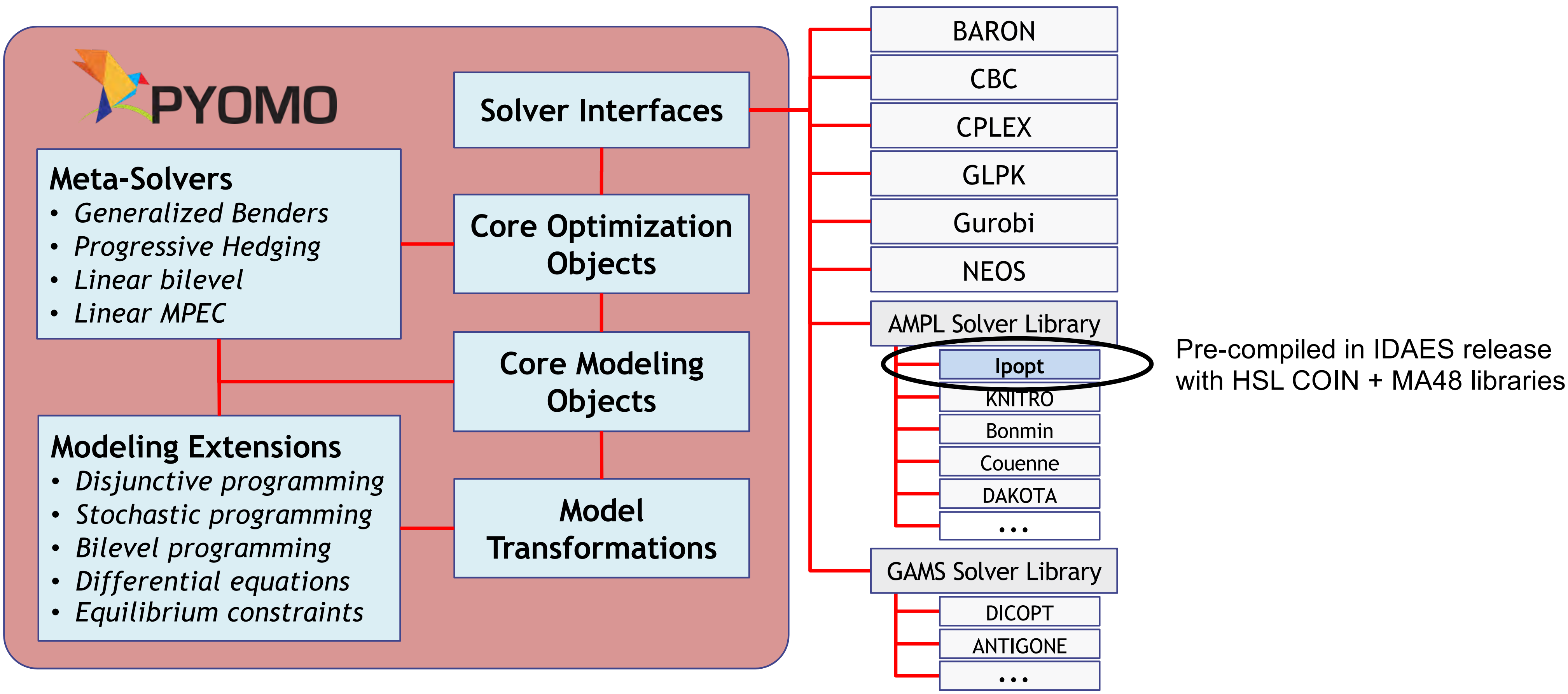
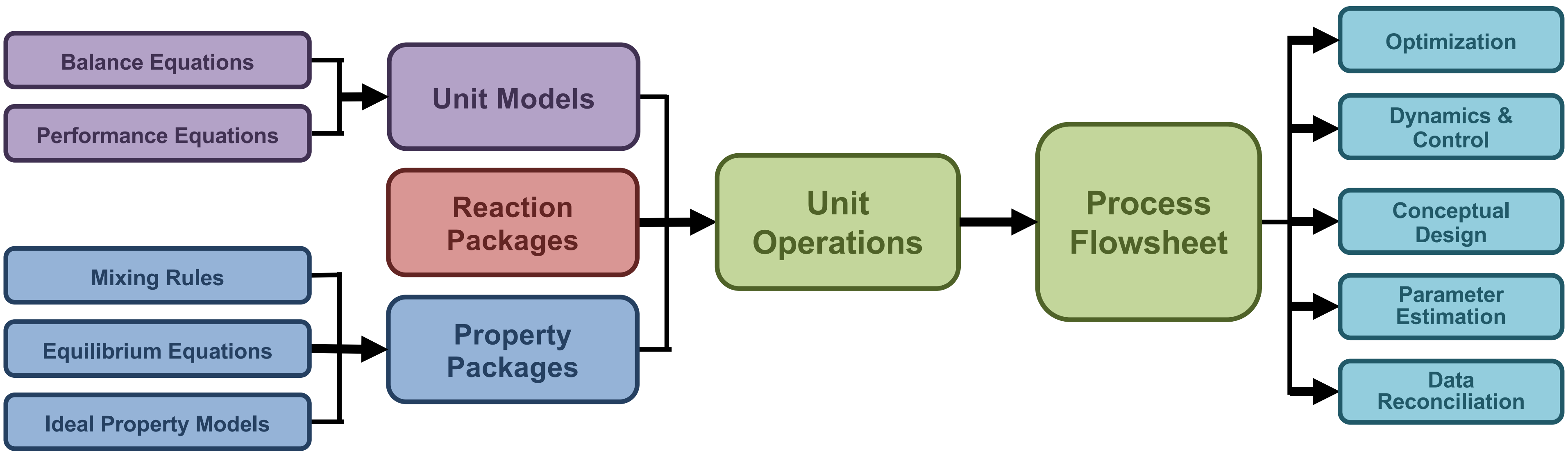
Pyomo: Python Optimization Modeling Objects



IDAES Model Structure

Flexibility and power of an equation-oriented modeling package

Supports the block structure of a process simulator



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Recent Applications and Impact

- Existing Plant Process Improvements & Optimization
- Design & Optimization of Complex, Interacting Systems
  - Design space exploration
  - Optimization of carbon capture systems
  - Robust design to reduce technical risk
- Bridging timescales between power plant and grid
  - Energy storage to reduce cycling / wear
  - Insights on optimal bid strategies to increase revenue

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Support for the Existing Coal-Generation Fleet

Partnership with Tri-State Generation and Transmission Association

Escalante Generating Station, Prewitt, NM

245 MW Subcritical Plant

Frequent Cycling

- Major focus areas
  - Reducing minimum load
    - Demonstrated 44% improvement upon correcting deaerator water hammer issue
  - Improving heat rate
    - Up to 2% improvement with a steeper sliding pressure approach to load following
  - Fault detection and diagnosis
    - Alarm settings can identify reheater plugging 4-5 days in advance (previously 1-2 days)
  - Extending equipment life
- Public releases
  - ✓ Jan 20: Steady-state power plant model library
  - ✓ July 20: Code for **data reconciliation**, **parameter estimation**, and **optimization**
  - Dec 20: Dynamic power plant model library

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IDAES Enables Complete Workflow from Analysis to Optimization

Data Reconciliation

"Ensure data is reliable"

$$\underset{\{temps, pressures, flows\}}{\textbf{Minimize}} \sum_{data} (error_{meas})^2$$

subject to

- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations

$$error_{meas} = \frac{\text{measurement} - \text{model prediction}}{\text{measurement uncertainty}}$$

Parameter Estimation

"Make models predictive"

$$\underset{\{parameters\}}{\textbf{Minimize}} \sum_{data} (error_{meas})^2$$

subject to

- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations
- Performance equations for unit models

System-wide Optimization

"Identify optimal operation"

$$\underset{\{temps, pressures, flows\}}{\textbf{Minimize}} \ Heat\ Rate$$

subject to

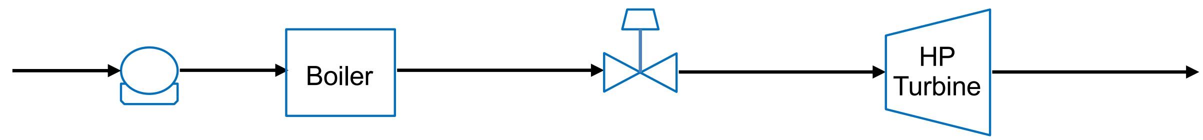
- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations
- Performance equations for unit models
- Load = Target Load
- Operational Constraints (e.g., $T<T_{max}$)
- Emissions < Emission Limits

System-wide Optimization Revealed Heat Rate Improvements Achievable through Steeper Sliding Pressure Operation

$$\underset{\{temps, pressures, flows\}}{\textbf{Minimize}} \quad \textit{Heat Rate}$$

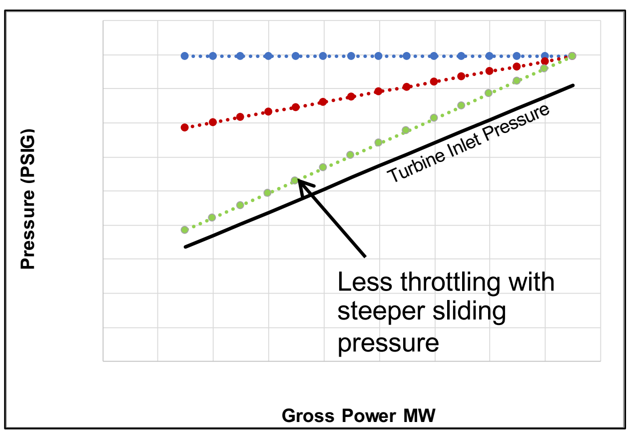
subject to

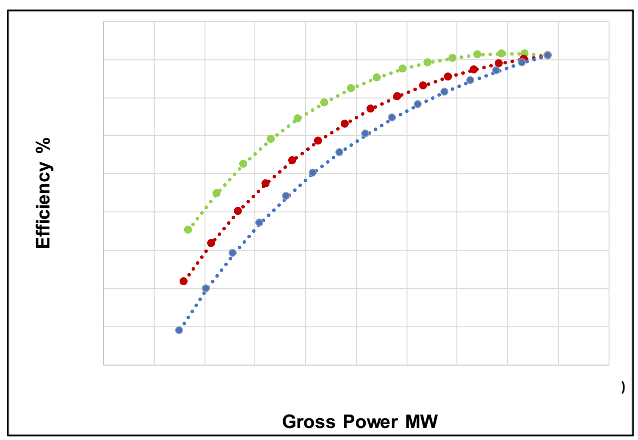
- Flowsheet connectivity
- Mass and energy balances
- Physical property calculations
- Performance equations for unit models
- Load = Target Load

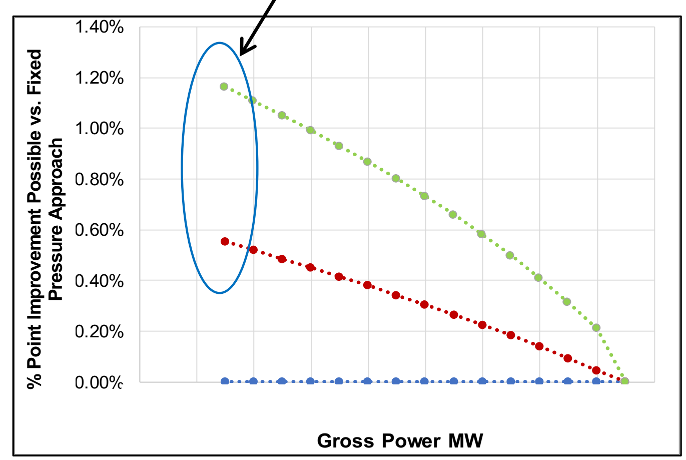


Main Steam Pressure:
- Fixed Pressure
- Current Operation
- Steeper Sliding Pressure

0.6 %-point (2% overall) improvement achievable with steeper sliding pressure







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  - Energy storage

Design & Optimization of Complex, Interacting Systems

Technology Selection ↔ **Optimal Design** ↔ **Transient Operability** ↔ **Grid Interactions**

Technology Selection

Conceptual Design
Physics based models
Reduced Order Models
NPV maximization

Optimal Design

Use rigorous models
Validate performance
Optimize design variables

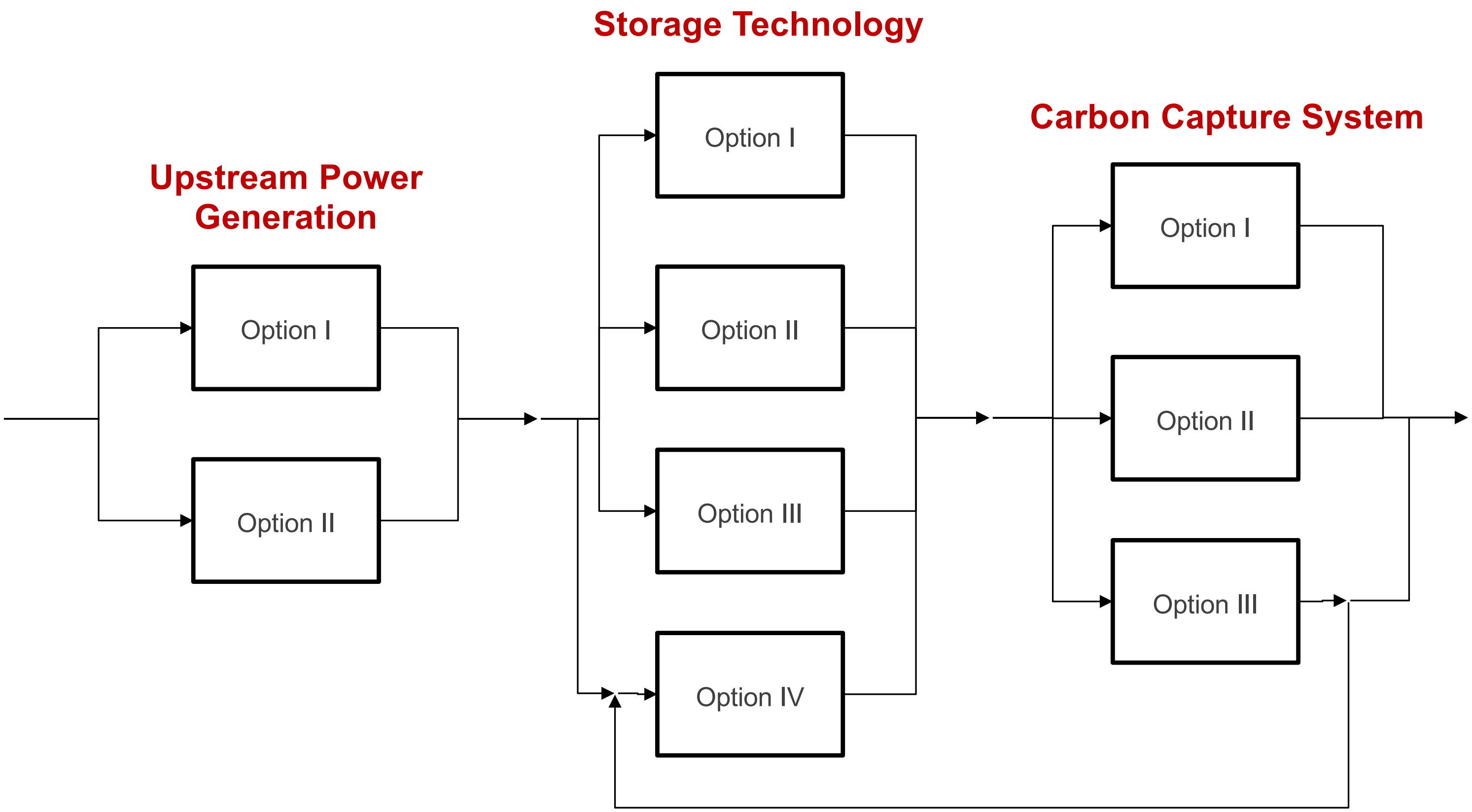
Transient Operability

Dynamic models
Control Design
Optimal plant dispatch
Identify operating constraints

Grid Interactions

Infrastructure Planning
Production Cost Model

Design Space Exploration of Options and Configurations



- Implement superstructure in IDAES
- Down select technologies faster
- Eliminate exhaustive TEA analysis for all possible configurations

9 disjunctions, 18 binary variables → 315 flowsheets to evaluate

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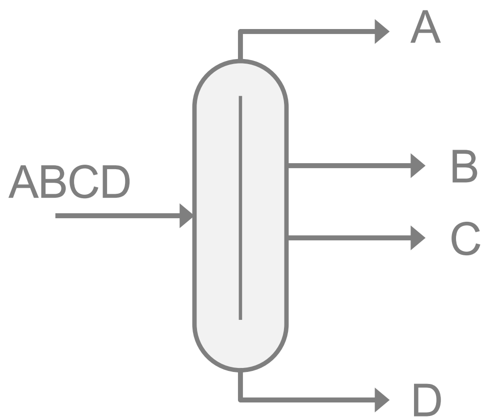
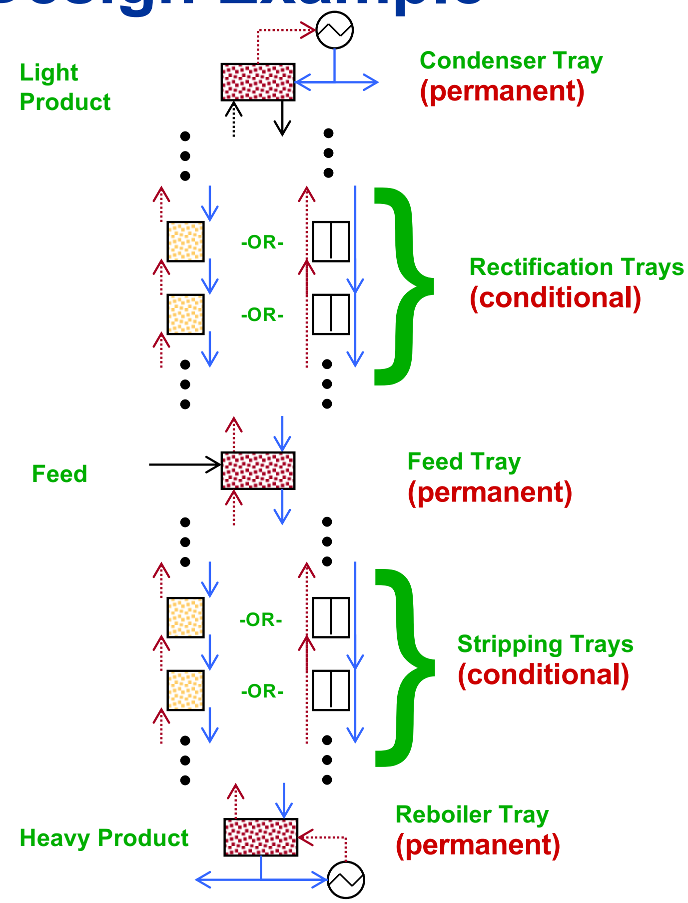
PyoSyn: Kaibel Column Conceptual Design Example

- **Components:** Methanol, ethanol, n-propanol, n-butanol
  - 99% purity for each component
- **42 million combinations**
- **GDP model written using Pyomo.GDP**
  - 5715 constraints
    - 2124 nonlinear
  - 100 disjunctions
    - 3599 variables
      - 178 binary
      - 3421 continuous
- **Solved in <u>639 sec using GDPopt-LOA solver</u>**
  - Logic-based outer approximation algorithm
  - **4 iterations**
- **Resulting design:**
  - **46 trays** (21% reduction vs. base case)
  - **Dividing wall between 12th and 26th tray**
  - **Feed at 18th tray**
  - **Side outlets at 13th and 22nd trays**

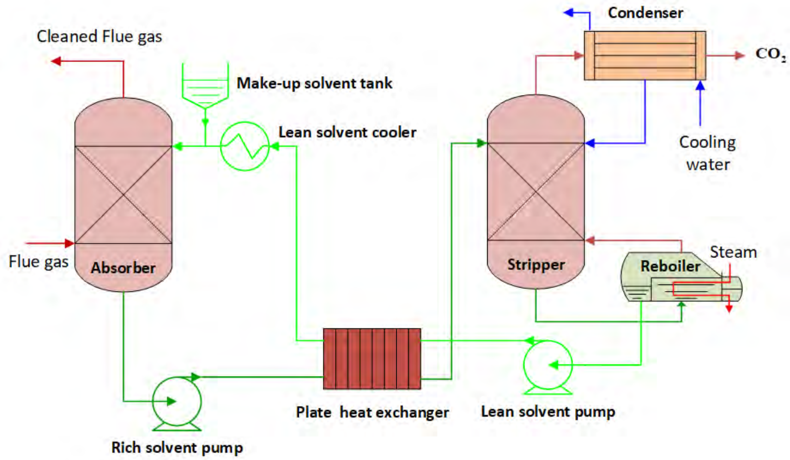




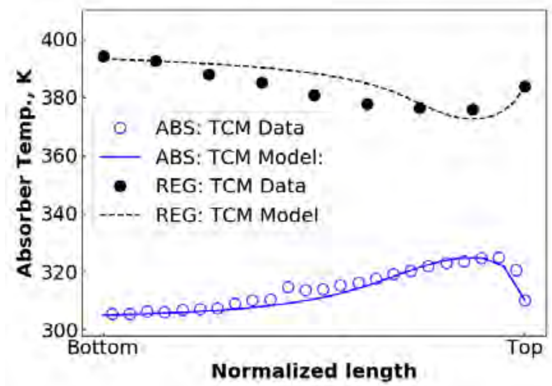
Optimal Design Kaibel Column <u>reduces energy consumption by more than 40%</u> compared to 2 columns

Rawlings, Chen, Grossmann, Caballero, Computers & Chemical Engineering, 125, 2019, 31-39.

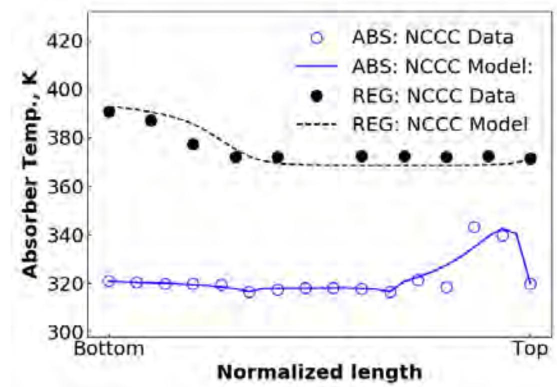
Amine-Based Post-Combustion CO_2 Capture Process



Model Validation Using TCM and NCCC Data

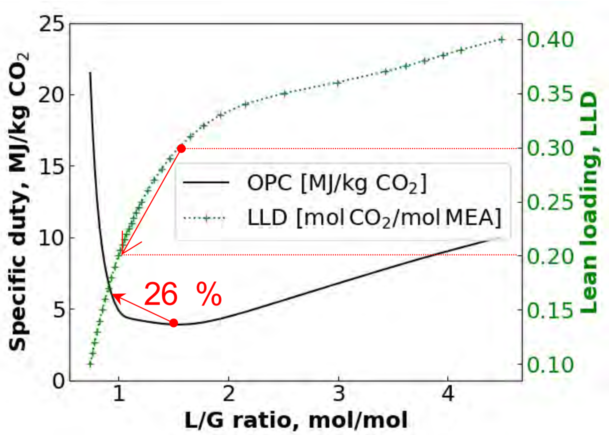


TCM



NCCC

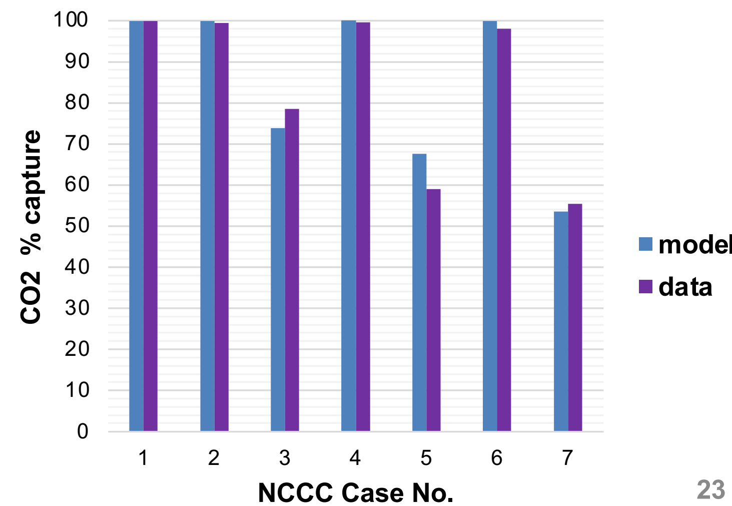
Process Optimization



- **Deviation from Optimal LLD**

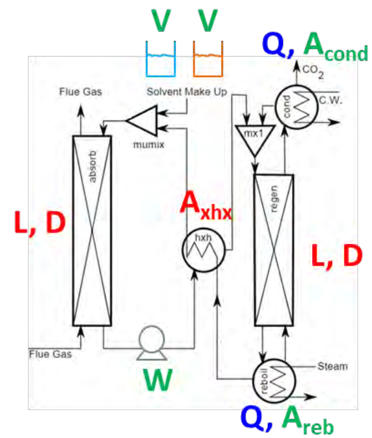
↓

- **Increase in Energy Cost**



PyROS: Robust Design CO_2 Capture System

- Design Variables (First-Stage)
  - Columns dimensions (D,A), heat exchanger areas (Axhx)
  - hold-up tank volumes (V), pump power (P)
- Control Variables (Second-Stage)
  - Duties (Qreb , Qcon)
- Uncertain Parameters
  - Equilibrium constant parameters (b1, b2)



Deteministic design fails to meet CO_2 capture performance requirement with a 33% probability

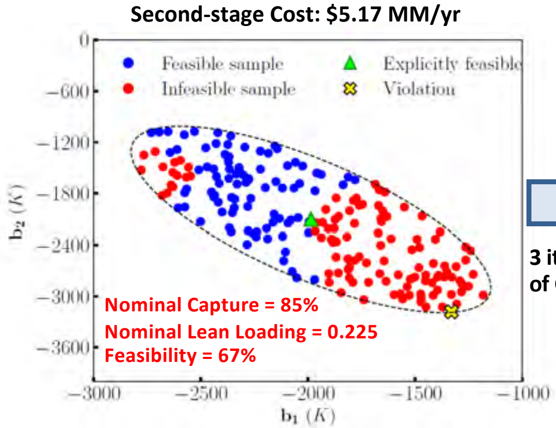
Robust design guarantees CO_2 capture in all scenarios; cost increase is kept to the minimum necessary to achieve this

Robustness achieved by increasing reboiler/condenser duties, which also lead to lower lean-loading (due to shorter regenerator column)

Deterministic Solution

Cost: \$7.37 MM/yr

Second-stage Cost: \$5.17 MM/yr



L_{abs} = 22.36 m D_{abs} = 2.84 m

L_{reg} = 12.29 m D_{reg} = 1.79 m

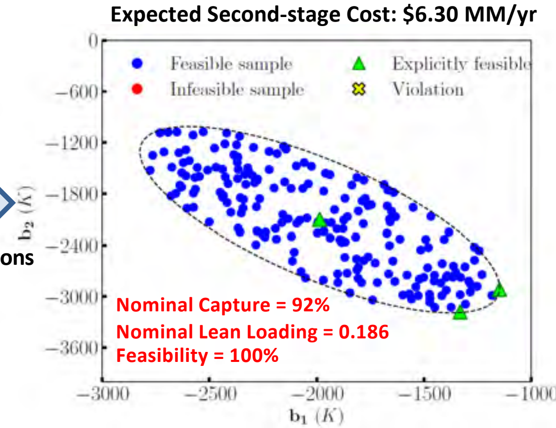
A_{xhx} = 6,688 m^2 Q_{reb} = 18 MW Q_{con} = -5.6 MW

3 iterations of GRCS

Robust Solution

Cost: \$10.82 MM/yr

Expected Second-stage Cost: \$6.30 MM/yr



L_{abs} = 17.04 m D_{abs} = 2.63 m

L_{reg} = 5.00 m D_{reg} = 2.47 m

A_{xhx} = 3,878 m^2 Q_{reb} = 23.5 $\pm$ 7.1 MW Q_{con} = -4.6 $\pm$ 7.7 MW

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Isenberg, N.. I., Akula, P., Eslik, J., Bhattacharyya, Miller, D. C. , Gounaris, C. E. (2020). Under Review.

Recent Applications and Impact

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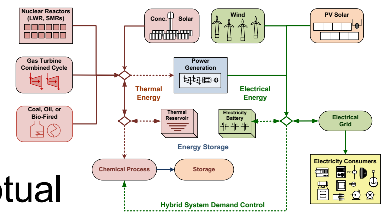
Bridging Timescales in IDAES Enables Unique Analyses

High-Fidelity Process Modeling

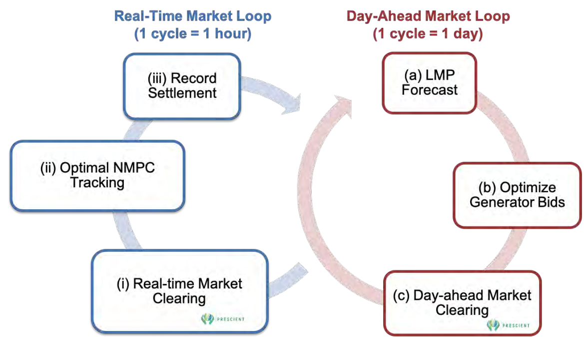
Dynamic Optimization and Control



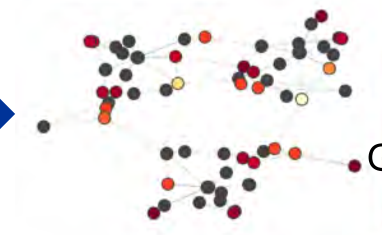
Conceptual Design

Data Reconciliation & Uncertainty Quantification

Resource-Grid Interactions



Grid Modeling



Expansion Planning

Grid / Market Simulation

PRESCIENT

1. Elucidate complex relationships between resource dynamics and market dispatch (with uncertainty, beyond price-taker assumption)
2. Predict the economic opportunities and market impacts of emerging technologies (e.g., Coal FIRST, tightly-coupled hybrid energy systems)
3. Guide conceptual design & retrofit to meet current and future power grid needs

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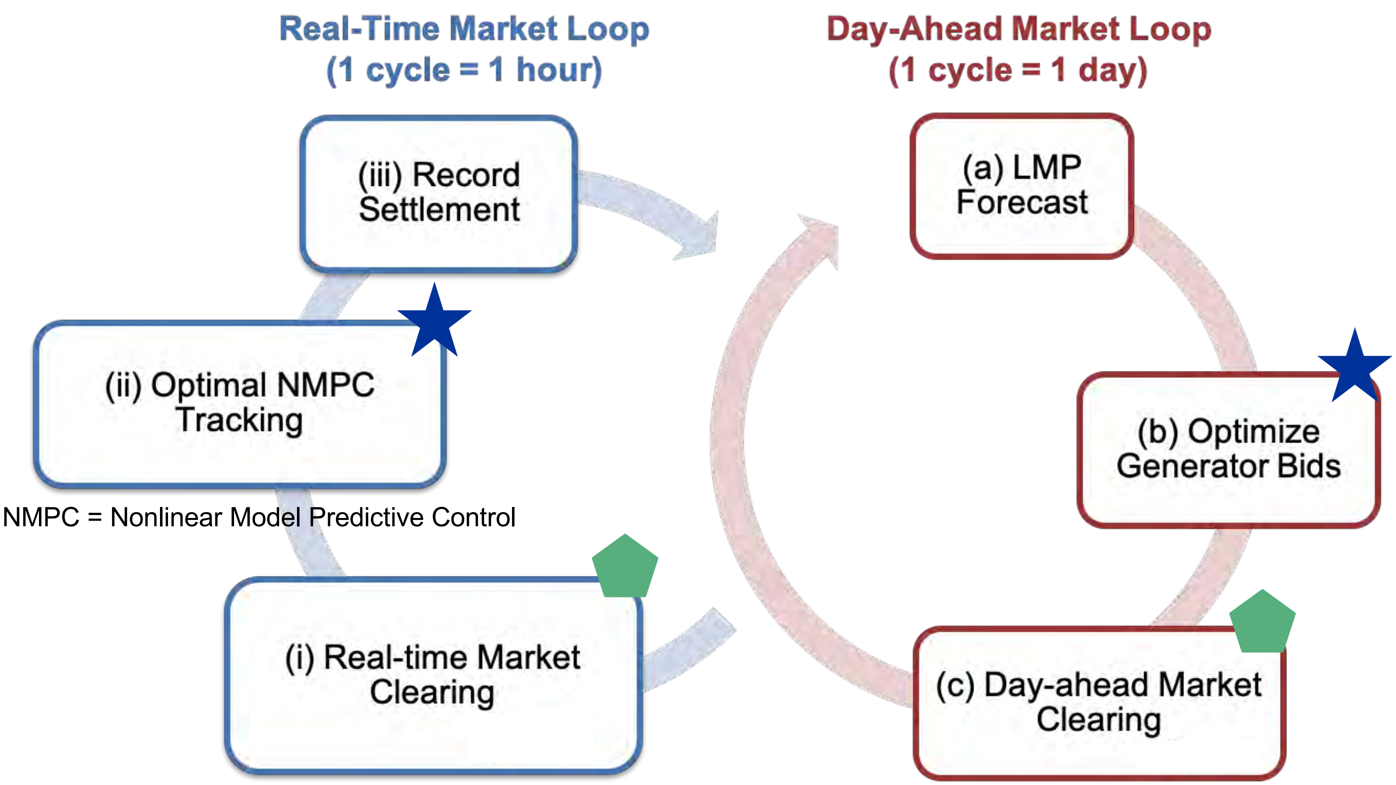
Modeling Multiscale Resource and Grid Decision-Making



★ Optimization problem(s) solved by resources (IDAES-PSE)

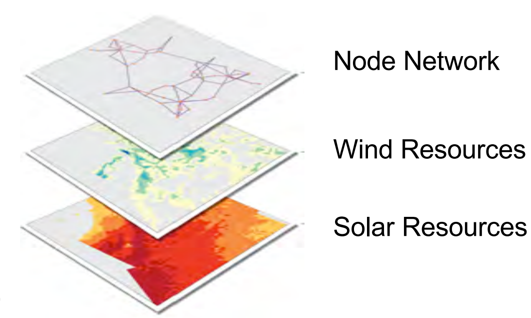
⬟ Optimization problem(s) solved by grid (Prescient)

PRESCIENT

Open source Production Cost Model (PCM)

Designed to closely mimic market clearing and settlement in U.S. electric markets

RTS-GMLC: open-source dataset developed by DOE to nominally mimic Southwest U.S.



https://github.com/grid-parity-exchange/Prescient
https://github.com/GridMod/RTS-GMLC

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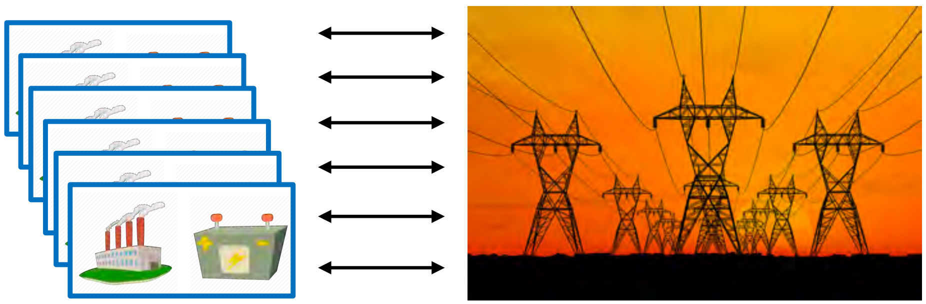
Thermal generators with energy storage

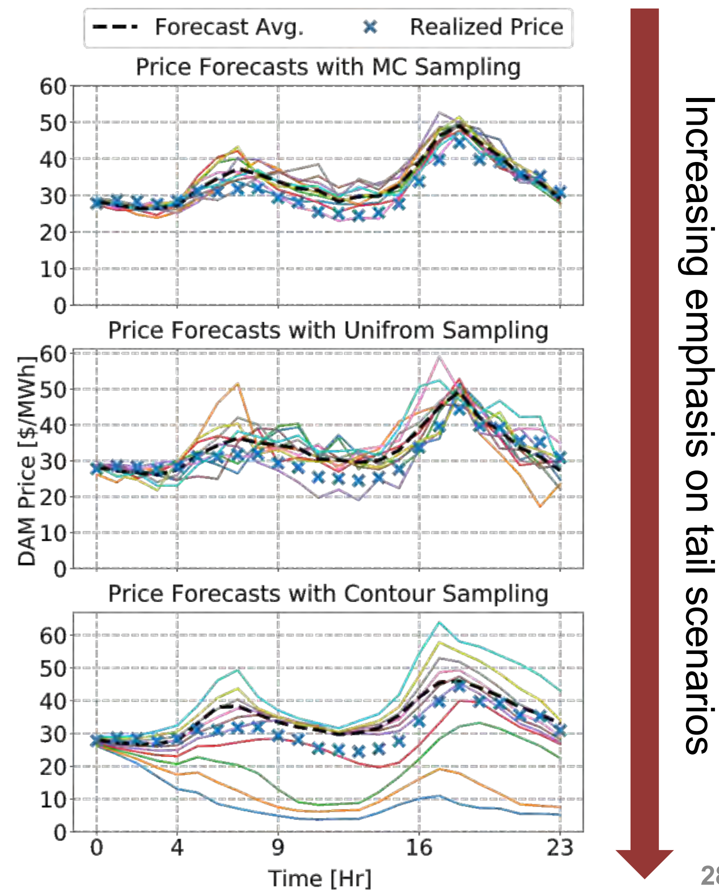
- Evaluate the impact of pairing thermal generators with electricity storage

Coal 1
Coal 2
CCGT 1
CCGT 2
Oil 1
Oil 2



- Optimize combined generator profit, subject to
  - Ramping limits
  - Minimum up/down time constraints
  - Storage energy balance
- Under two operating modes:
  - Self-schedule
  - Bidding

Forecast: Sampling strategies



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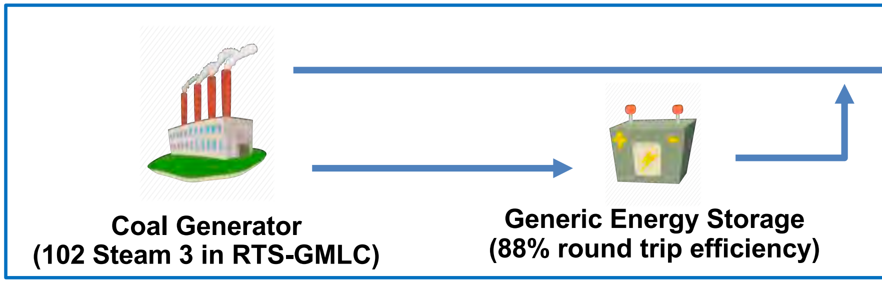
Quantifying the opportunity of integrated analysis

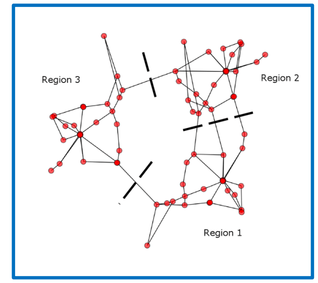
Model	Participation Mode	Perfect Information (M$)	MC Sampling (M$)	Uniform Sampling (M$)	Contour Sampling (M$)
Thermal Generators	**Bid Curve**	51.8 (100%)	46.2 (89.3%)	47.3 (91.3%)	47.5 (91.7%)
	Self-schedule		42.1 (81.3%)	41.0 (79.2%)	41.3 (79.6%)
Thermal Generators + Storage	**Bid Curve**	54.1 (100%)	46.6 (86.2%)	48.2 (89.0%)	47.9 (88.6%)
	Self-schedule		43.6 (80.5%)	41.3 (76.3%)	42.5 (78.5%)

Bidding (direct market participation) is more robust to market price uncertainty.

Hybrid system tracked market dispatch with 30% less ramping

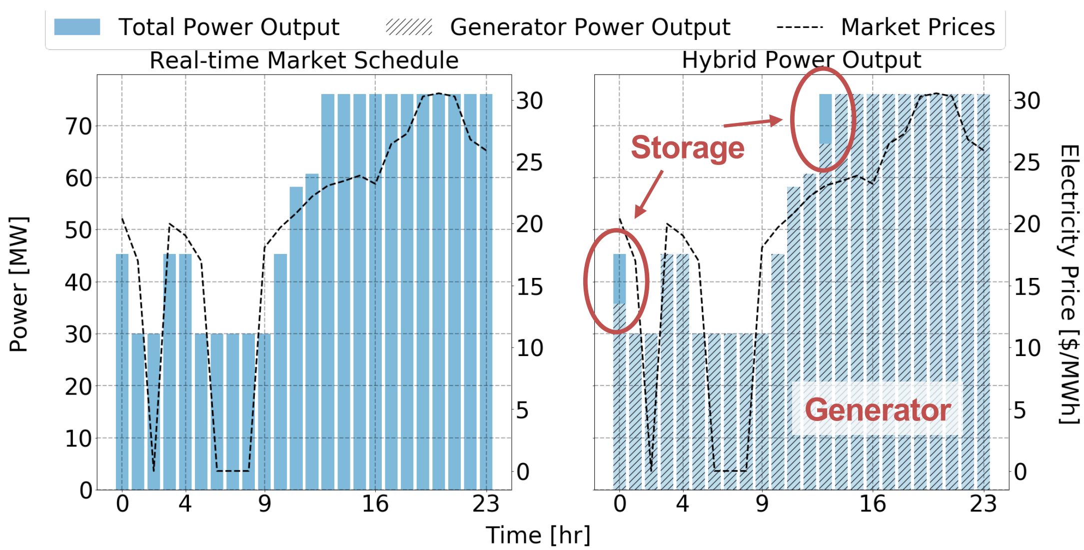
Idealized Hybrid System





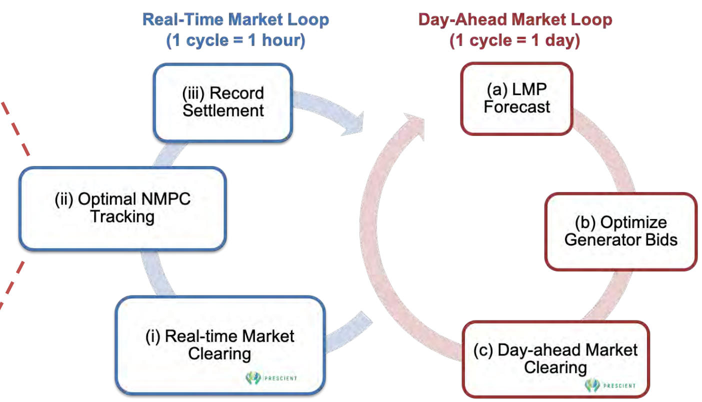
Electricity Grid / Market

(RTS-GMLC System)



Market Dispatch

Optimal Operating Policy



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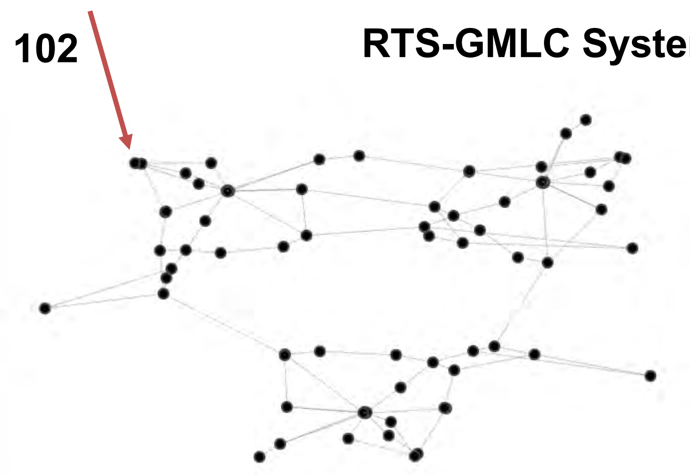
Optimize Bidding Strategy for Coal Steam 3 Generator

Steam 3 Generator

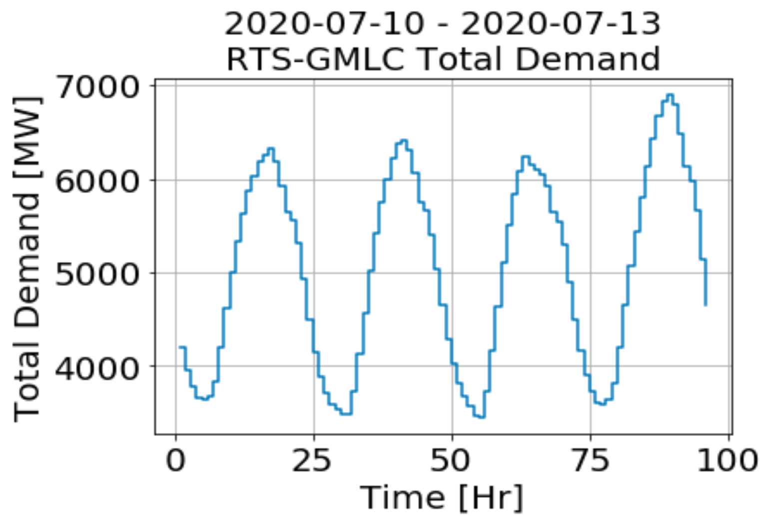
76 MW
32.6% efficient (full capacity)

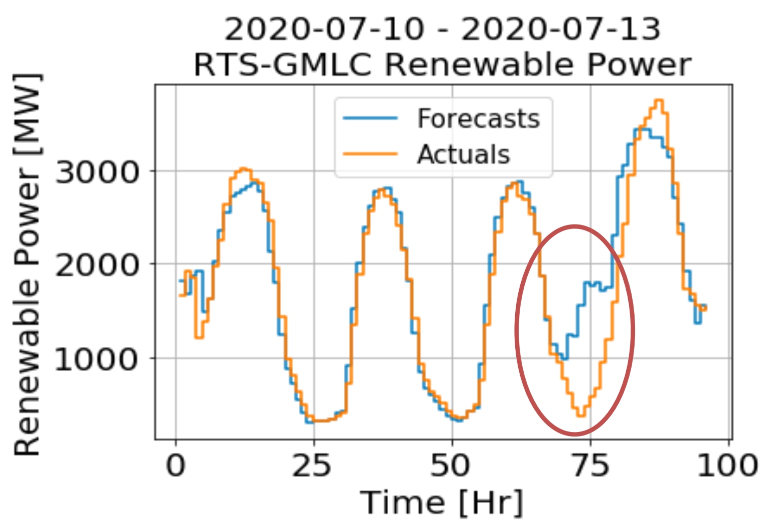
Bus 102

RTS-GMLC System



158 generators (42% dispatchable)
14,550 MW capacity (54% dispatchable)





Large Shortfall in Renewable Power on Day 3 @ 11pm

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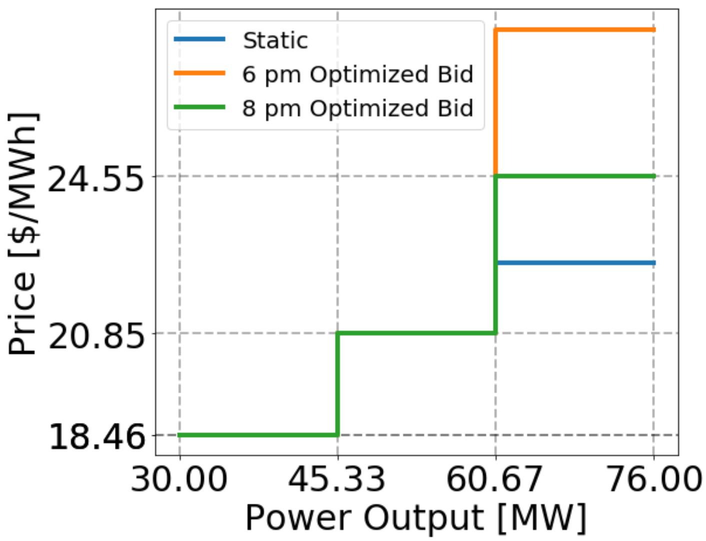
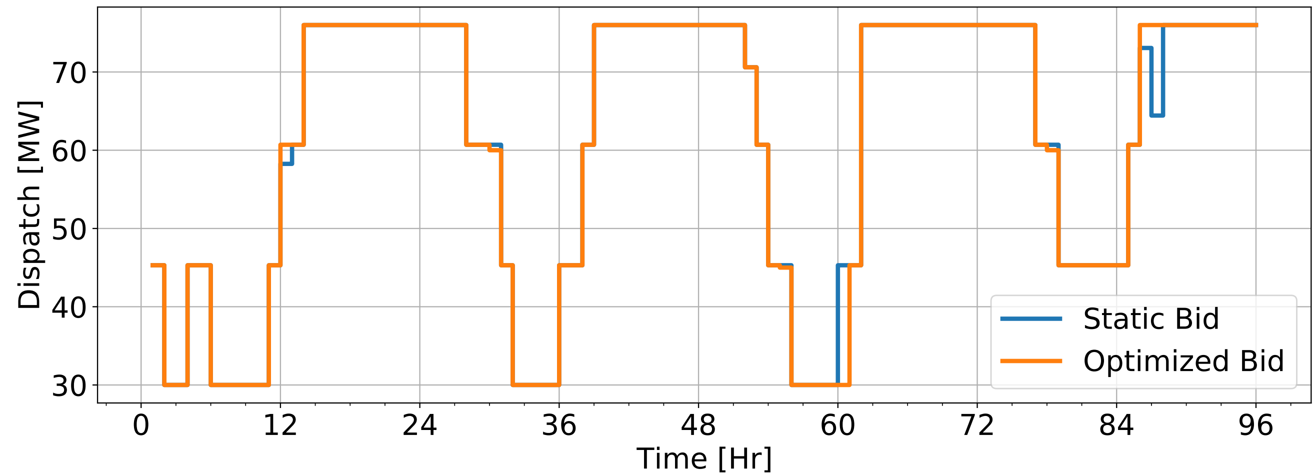
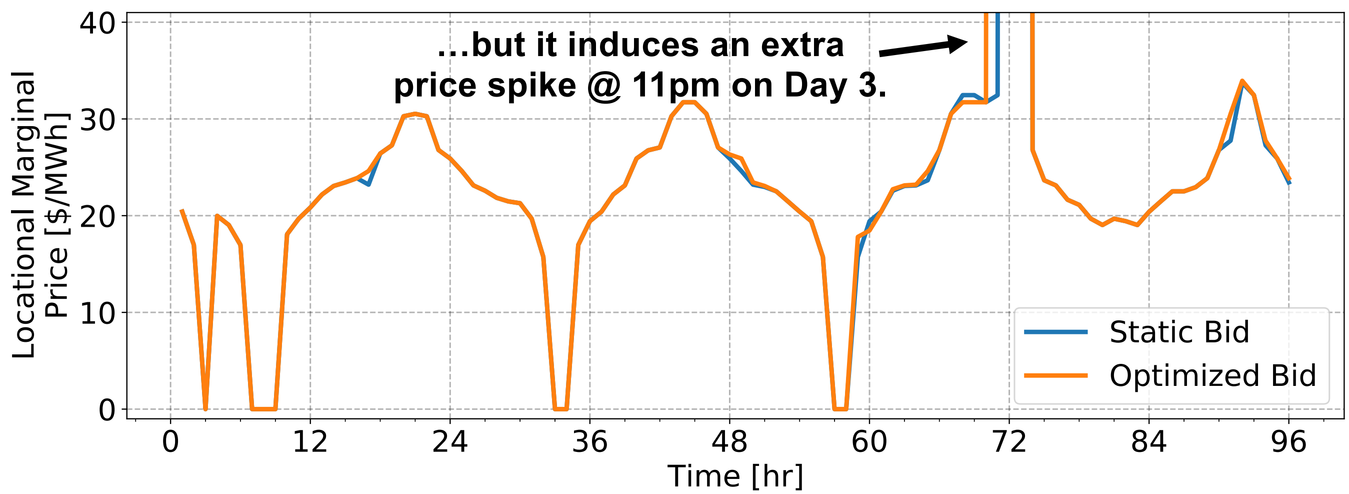
Data: RTS-GMLC, https://github.com/GridMod/RTS-GMLC

Optimal Bid Changes Dispatch & Increases Revenue

Optimizing the bid curves for 102 Steam 3 generator causes only minor changes in its dispatch schedule from the market…







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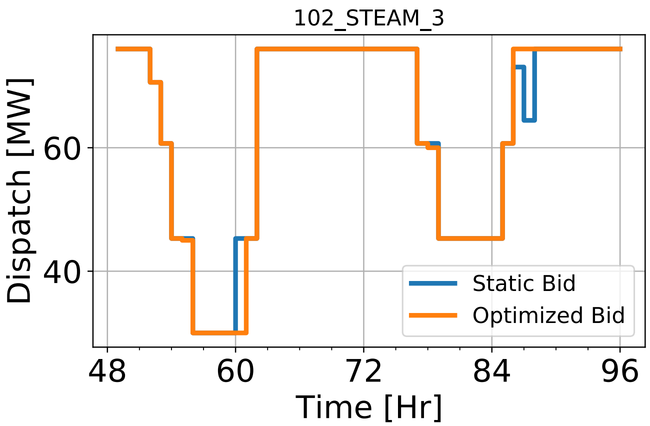
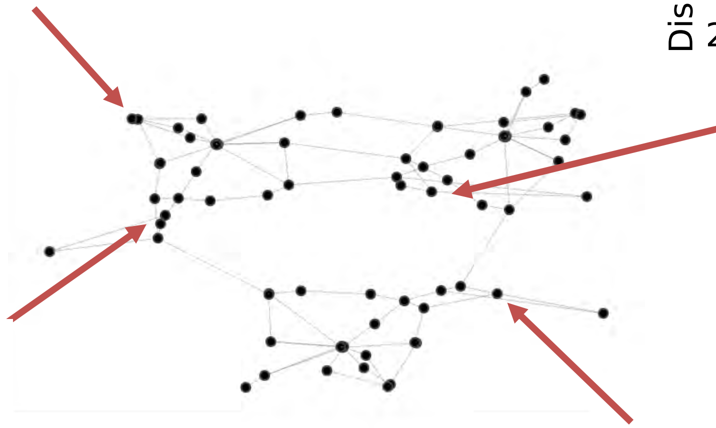
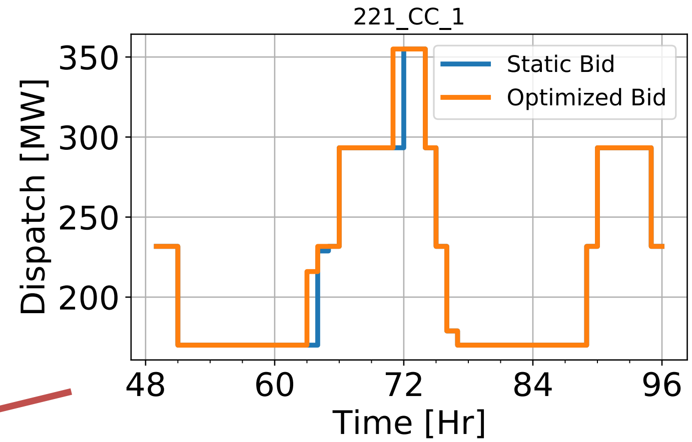
Changes in a single generator impacts entire network

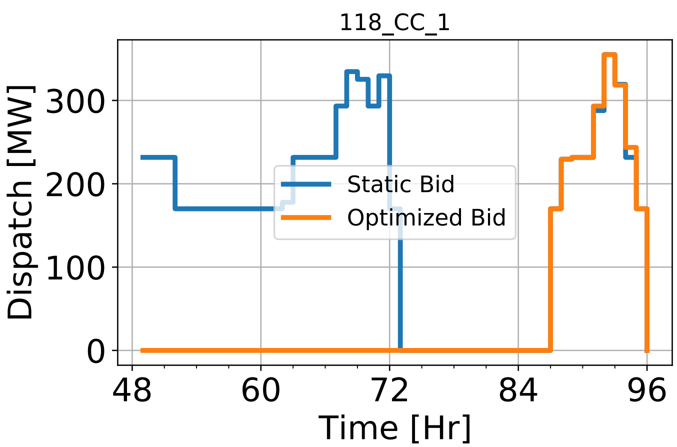


There is a shortfall at 11pm (not enough generation) which cases the price spike.

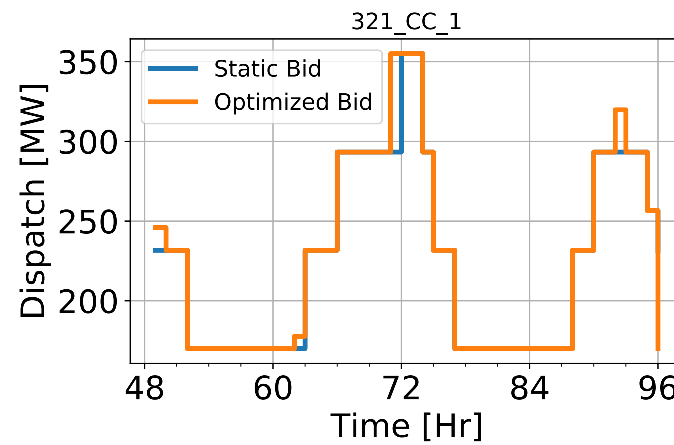




Combined Cycle plants at Busses 221 and 321 are dispatched at 100% at 11pm.



Combined Cycle 1 plant at Bus 118 is OFF in Day 3.



Conclusions: Recent Applications and Impact

- Existing Plant Process Improvements & Optimization
  - Improved minimum operating load by 44%
  - Opportunity to increase overall efficiency by 2%
- Design & Optimization of Complex, Interacting Systems
  - Design space exploration
    - Reduced energy demand by >40% through automated exploration of 42 million alternatives
  - Optimization of carbon capture systems
    - Reduced operating cost by 15-18%
  - Robust design to reduce technical risk
    - Inherently robust against uncertainties in the core process thermophysical properties
- Bridging timescales between power plant and grid
  - Energy storage
    - Increased revenue opportunities
    - Reduced equipment wear and tear by >30%
  - Insights on optimal bid strategies to increase revenue
    - Captures complex interactions among generators & bulk power market
    - Analysis of emerging flexible energy systems must capture interactions with the balance of the grid

Extended Applications of IDAES

National Alliance for Water Innovation

CHANGING WHAT'S POSSIBLE

GRID MODERNIZATION LABORATORY CONSORTIUM
U.S. Department of Energy

Virtual Joint Stakeholder Workshop

- October 1 @ 11-2:15 Eastern
  - Plenary presentations
- October 8 @ 11-1:20 Eastern
  - Topical presentations
- October 15 @ 11 – 1:20 Eastern
  - Topical presentations

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CCSI²
Carbon Capture Simulation for Industry Impact

Available Videos and Tutorials

- **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.org

github.com/IDAES/idaes-pse

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