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SAND2020-3061PE

Applications Driving IDAES Process Systems Engineering Framework Capabilities

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March 9, 2010

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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
  - Extensible property packages
  - Initialization schemes
  - Numeric methods
    - Numerical methods on GPUs
    - Robust optimization for process systems
  - Custom system models
    - Chemical looping combustion
    - Dynamic two-film tower model for an electrolyte system
    - Stress and fatigue analysis
  - 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)
  - Electric grid integration
    - Capacity expansion planning
    - Market modeling and simulation (Prescient)
  - Systems integrationMaterials design
    - Optimization-based materials design

- The IDAES-PSE Framework 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.

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IDAES and the CAPD Annual review

- Many of the capabilities in IDAES are being developed by the CAPD
  - And will be featured in various talks and posters

- This talk will focus on three applications IDAES has been developing:
  - Providing support for the existing fleet of coal-fired power plants
  - Design of new generation systems and the Coal FIRST initiative
  - Modeling the interactions between generation systems and the power grid

Part 1: Supporting 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
  - Improving heat rate
  - Fault detection and diagnosis
  - 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

Blue hats: IDAES team

White hats: Tri-State R&D

Yellow hats: Escalante operators and engineers

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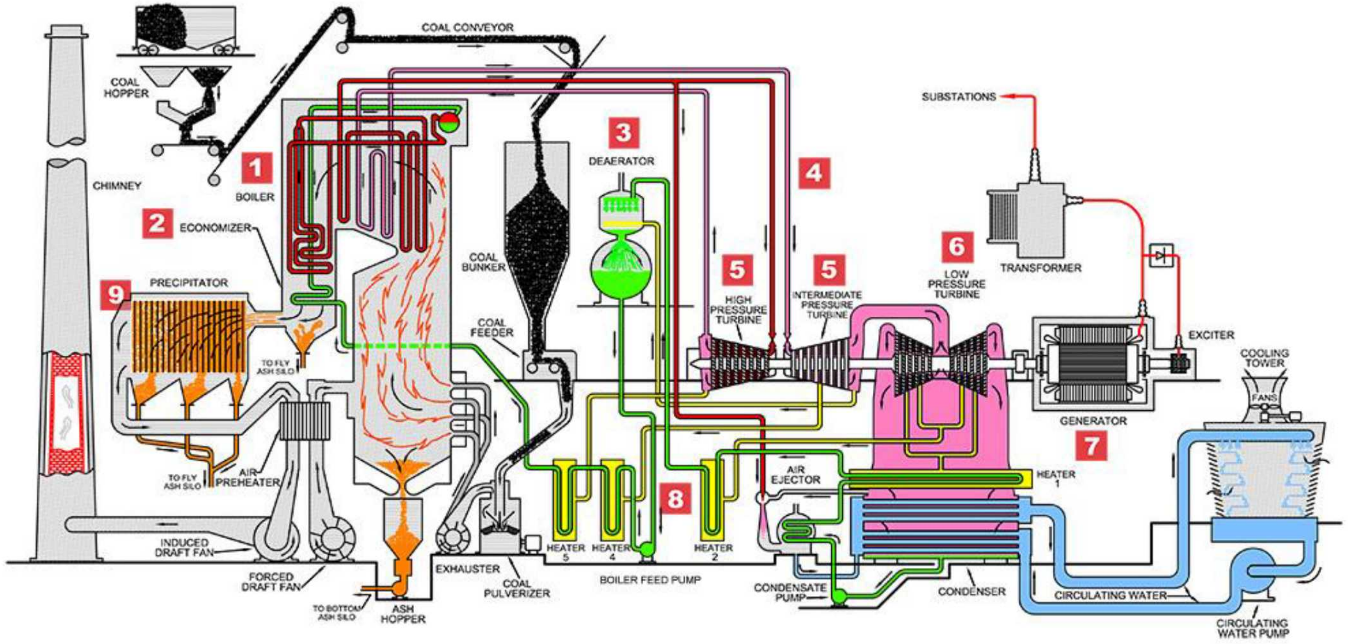
Power Plant Modeling and Optimization Capabilities



Source: Electric Power Research Institute, "Primer on Flexible Operations - 3002000045," EPRI, Palo Alto, Ca, September 2013

- Usable PSE framework for constructing optimization-ready process models
- Steady-state power plant optimization model
  - Boiler fire side (combustion, NO_x, SO_x formation)
  - Boiler water side (vertical tubes, convective superheaters, economizer)
  - Steam cycle (turbines, condenser, feedwater heaters, deaerator, pumps)
  - Pollution controls (SCR, FGD)
- Key features
  - Suitable for optimizing baseload & part load conditions
  - Rigorous physical properties calculations (e.g., IAPWS-95 for water and steam, must handle phase change)
  - Hybrid 1-D/3-D zonal model of boiler fire-side
  - Fully equation-oriented models for rest of flowsheet
- Established workflows for
  - Data reconciliation
  - Parameter estimation
  - System-wide optimization
  - Fault detection and diagnosis

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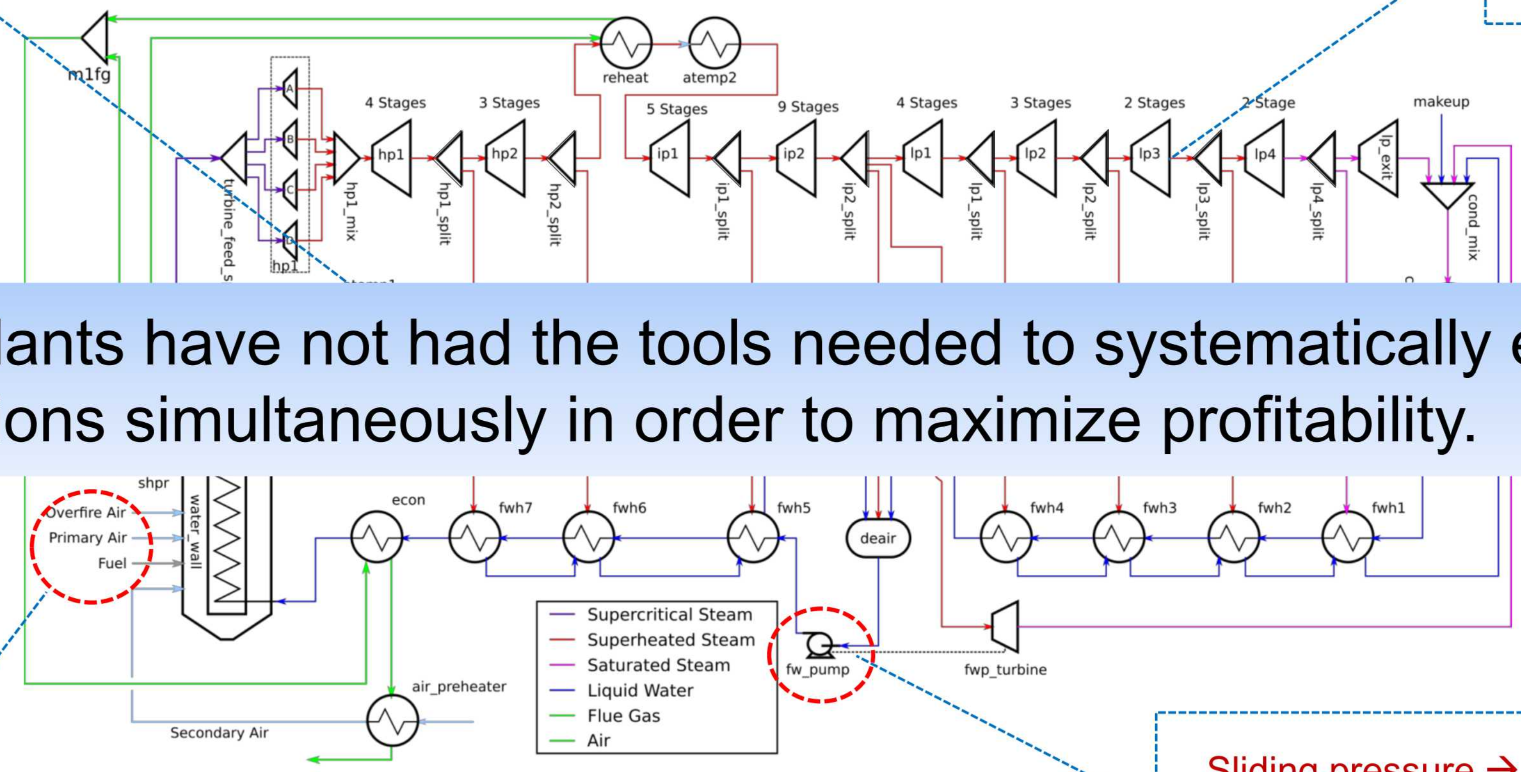
System-wide Optimization of Power Generation

Fixed pressure
→ Fix pressure of BFW in boiler but change pressure at turbine inlet

Steam extraction rates (at full and partial loads)



Typical power plants have not had the tools needed to systematically evaluate all options simultaneously in order to maximize profitability.

Coal firing rate

Simplified Example Flowsheet
(not Escalante's topology)

Sliding pressure → Change pressure of BFW in boiler

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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

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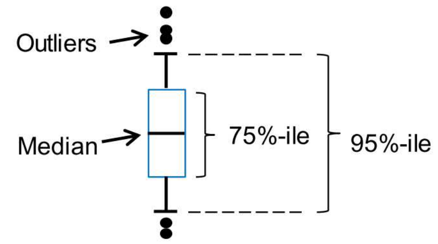
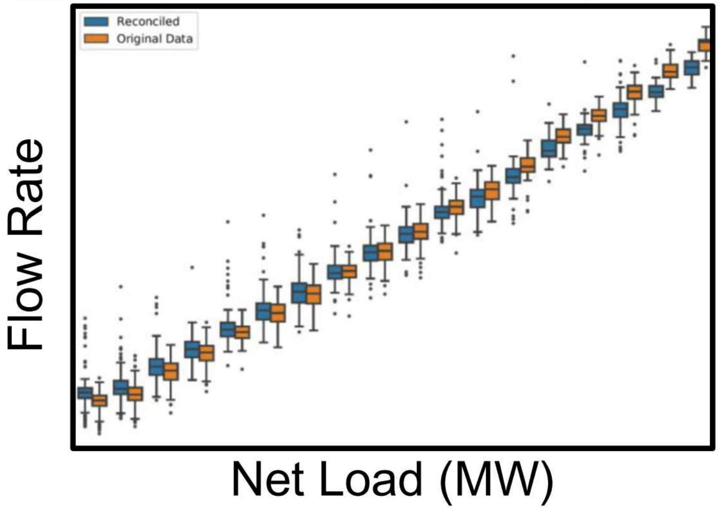
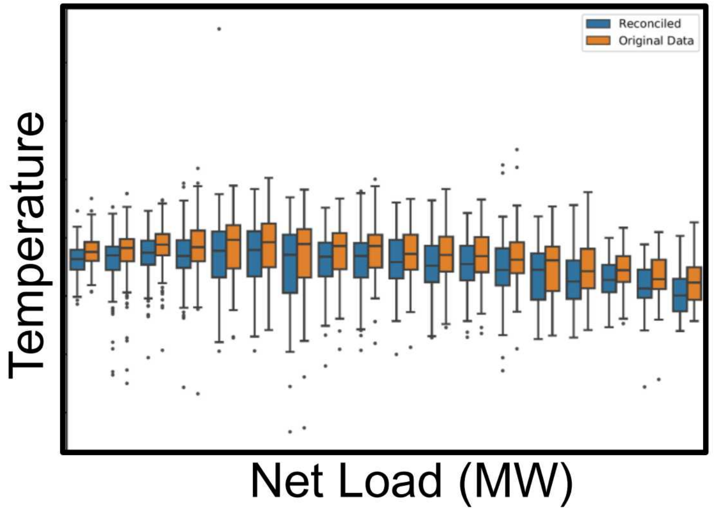
Data Reconciliation Allows Characterizing Uncertainty in Measured and Unmeasured Quantities

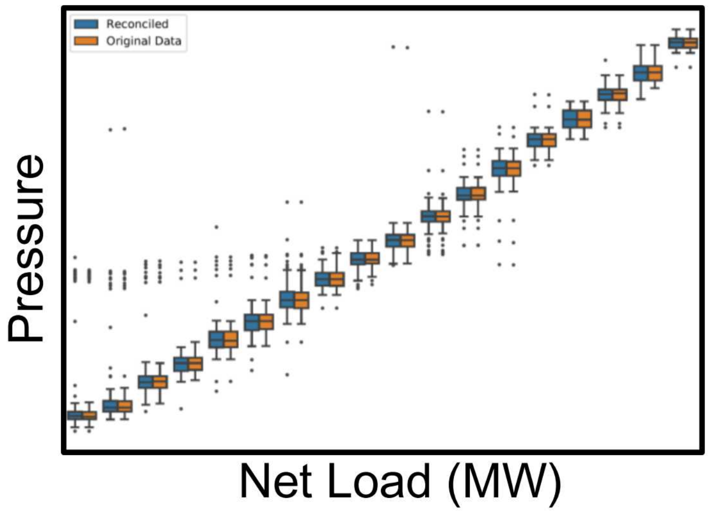


Hourly data: Jan 10, 2019 – Apr 8, 2019

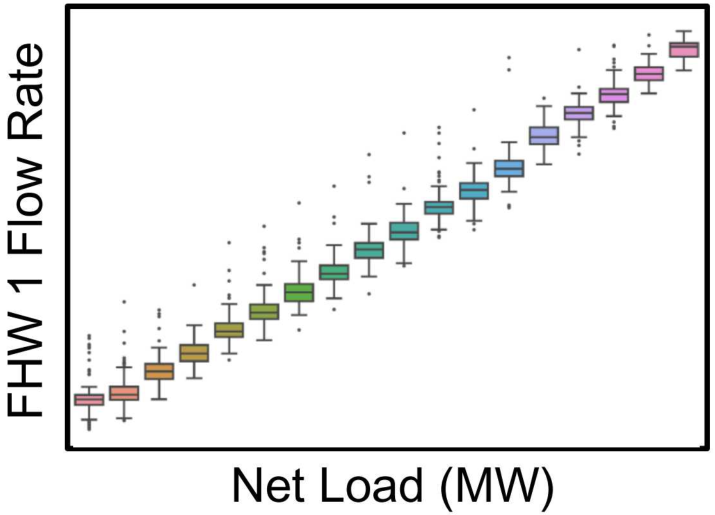
Main Steam Measurements (Measured)

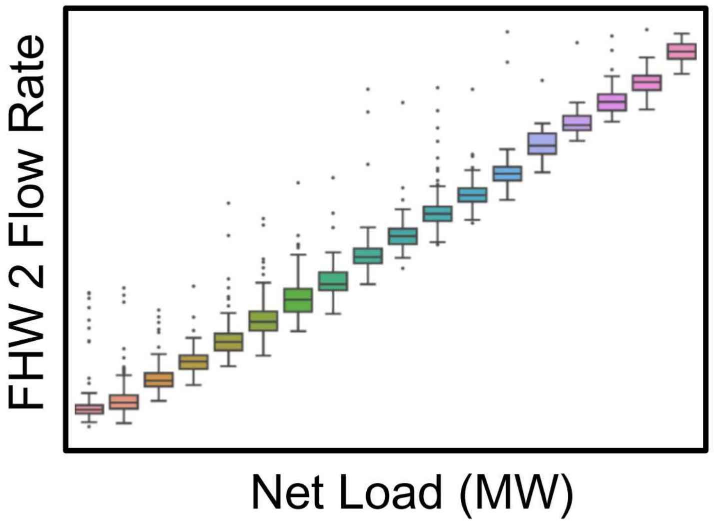


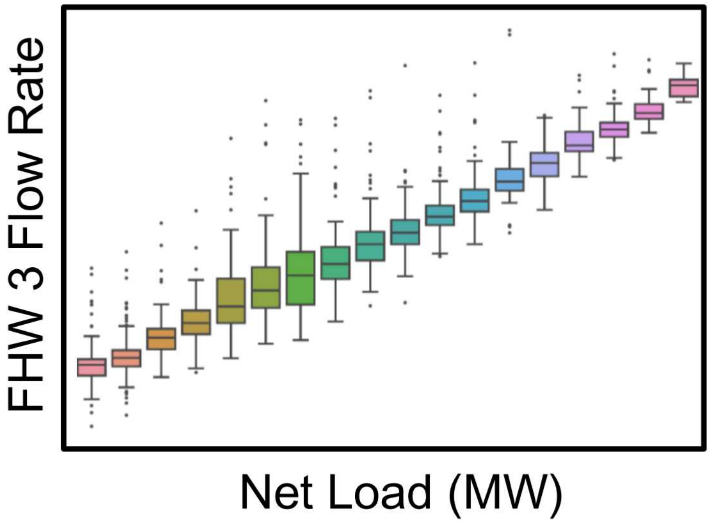




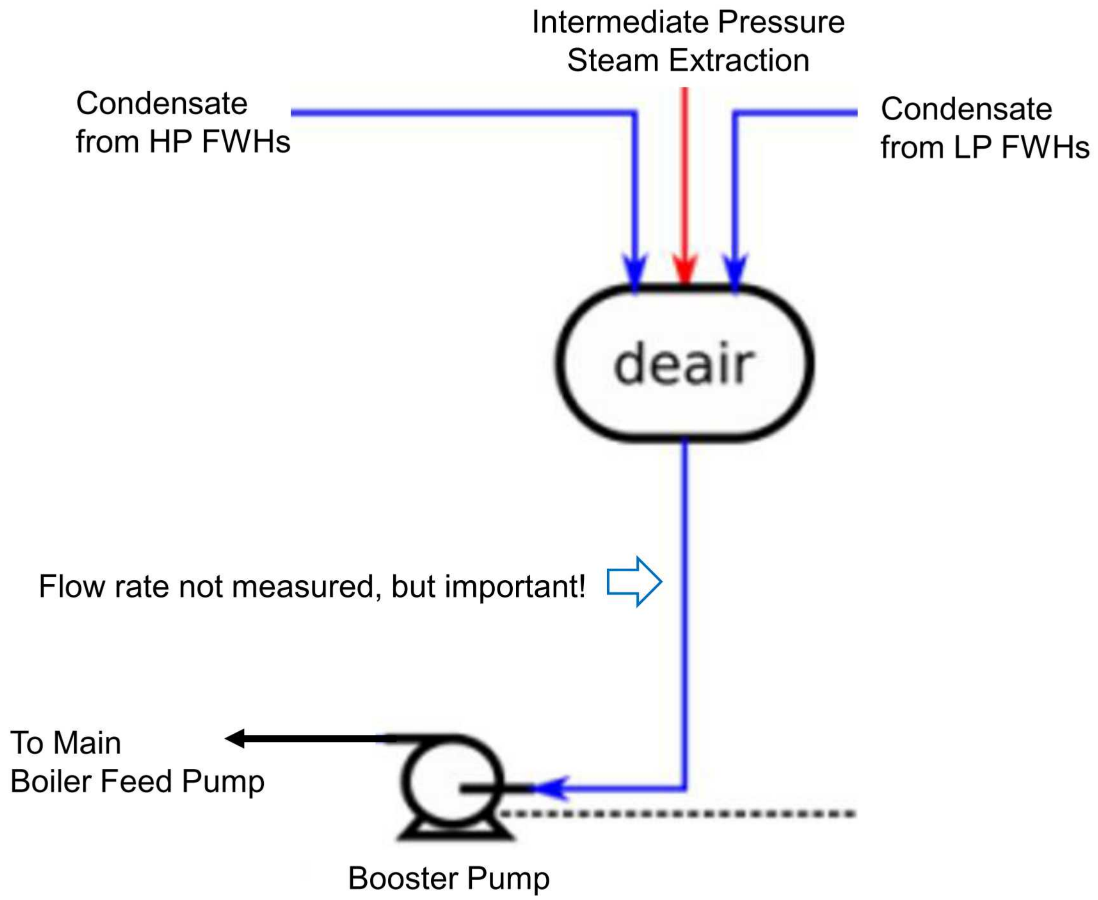
Steam extraction flow rates (Not Measured)

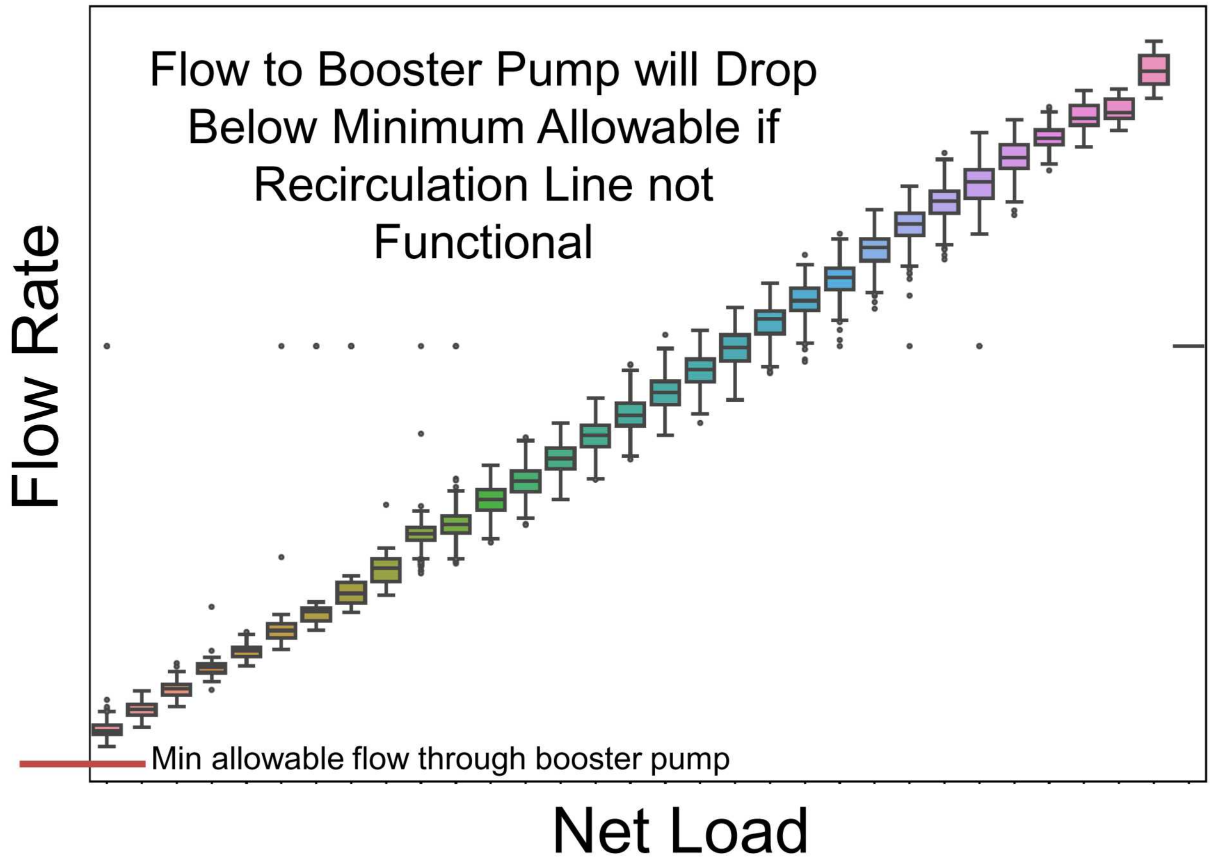






Data Reconciliation Enabled Diagnosis of Minimum Load Bottleneck





Six new flow meters were installed at Escalante primarily to support this work.

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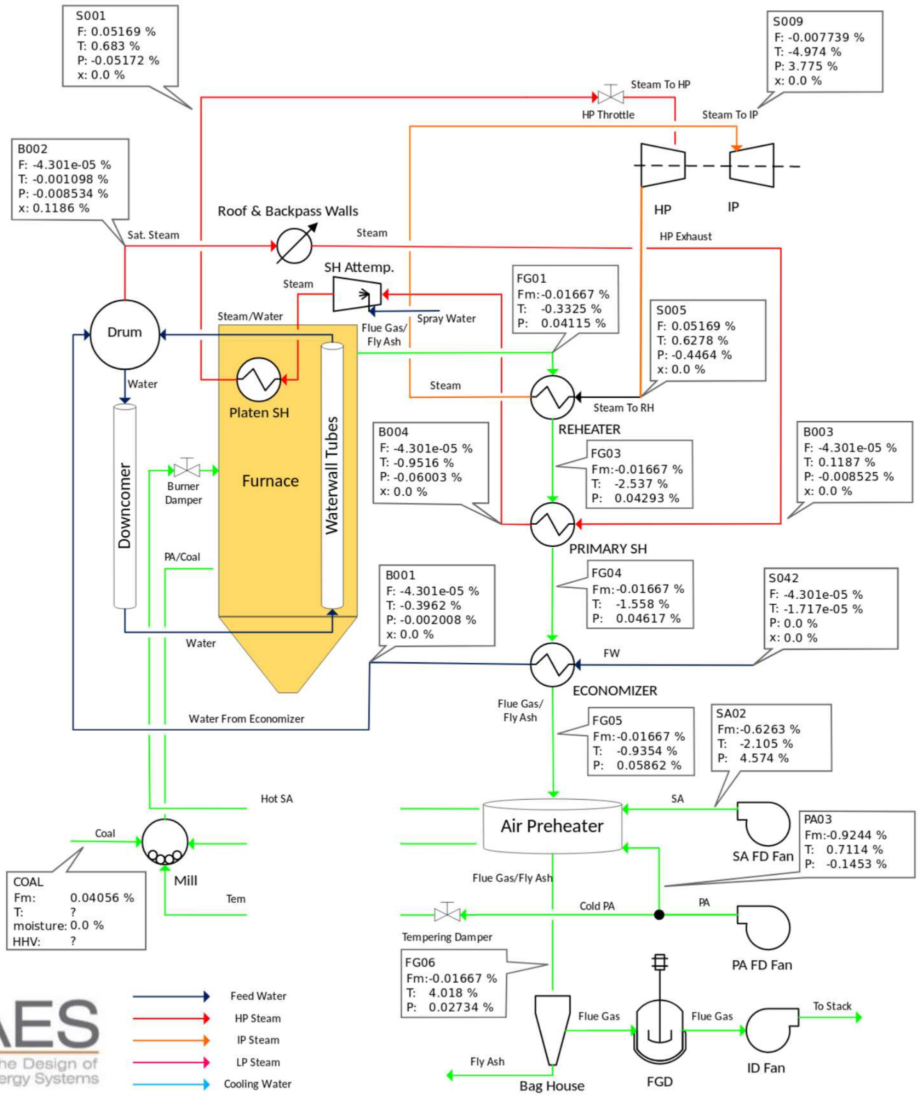
Parameter Estimation Required to Generate Models Predictive Enough to Make Meaningful Recommendations



Estimated Parameters

- Shell and tube heat transfer correction factors
- Shell and tube pressure drop correction factors
- Pipe pressure drop correction factor
- Water wall tube slag thickness

Mathematical Model

- 1800 variables, 1784 equations
- Solver: IPOPT
- CPU Time: 40 s (set-up, initialize, & solve)

< 1% model prediction errors in key quantities

See Zamarripa, et al, IDAES Data Reconciliation and Parameter Estimation Frameworks (CAPD poster)

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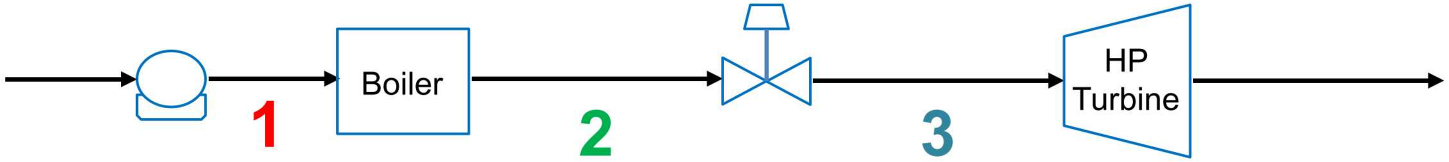
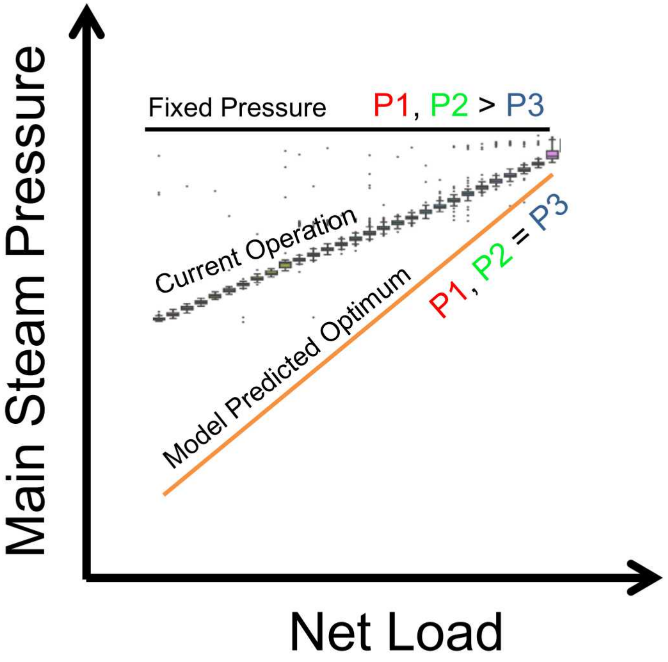
System-wide Optimization Revealed Heat Rate Improvements Achievable through Steeper Sliding Pressure Operation

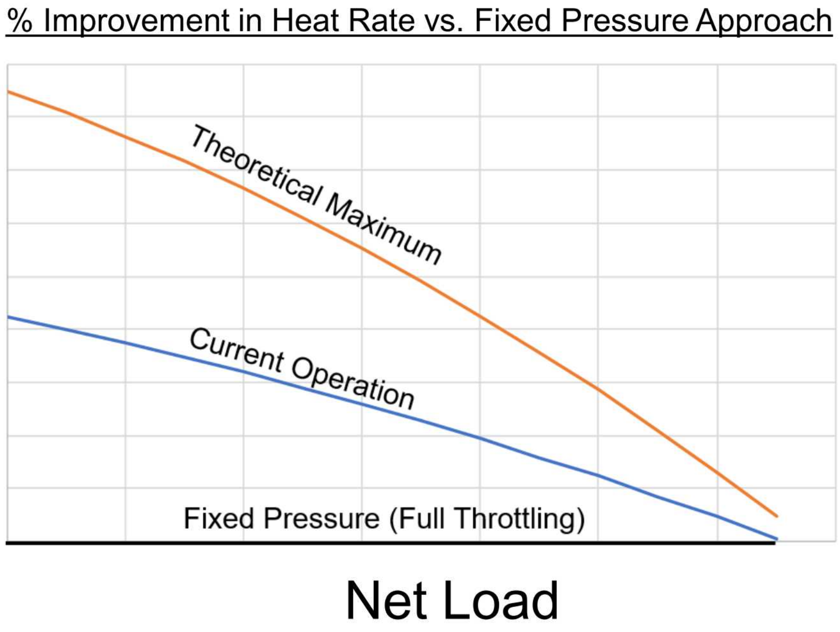


$$\underset{\{temps, pressures, flows\}}{\textbf{Minimize}} \quad Heat\ Rate$$

subject to

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





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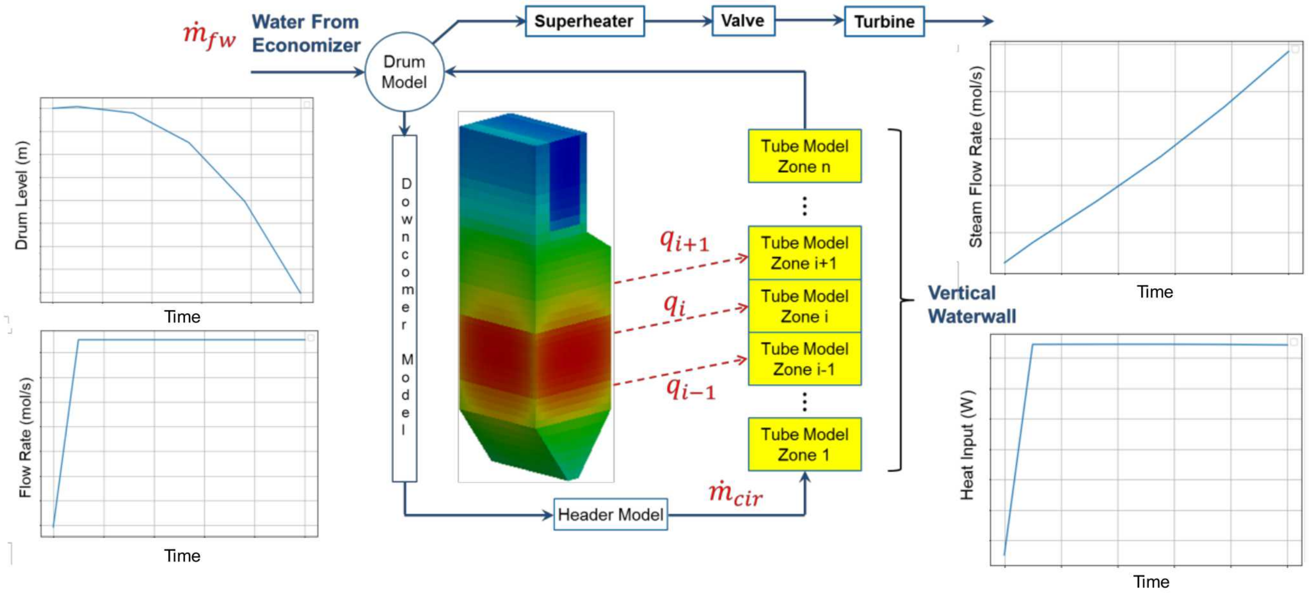
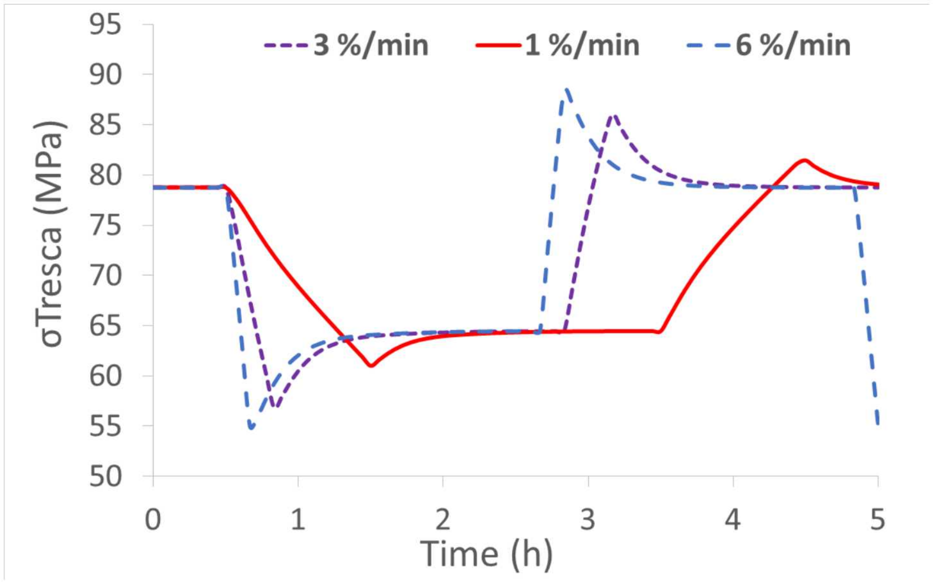
Coupling Dynamic Models with Fatigue/Damage Models to Quantify Impact of Load Following





Ref: ramp rate 3%/min
N: number of cycles before a failure is likely to occur**

See Nicholson, et al, Dynamic Modeling and Optimization of Advanced Energy Systems (CAPD poster)

Steam Drum

- Drum material: **SA 299**

	1 %/min *	3 %/min	6 %/min
N**(Times)	2.68×10^{11}	4.21×10^{9}	1.30×10^{9}

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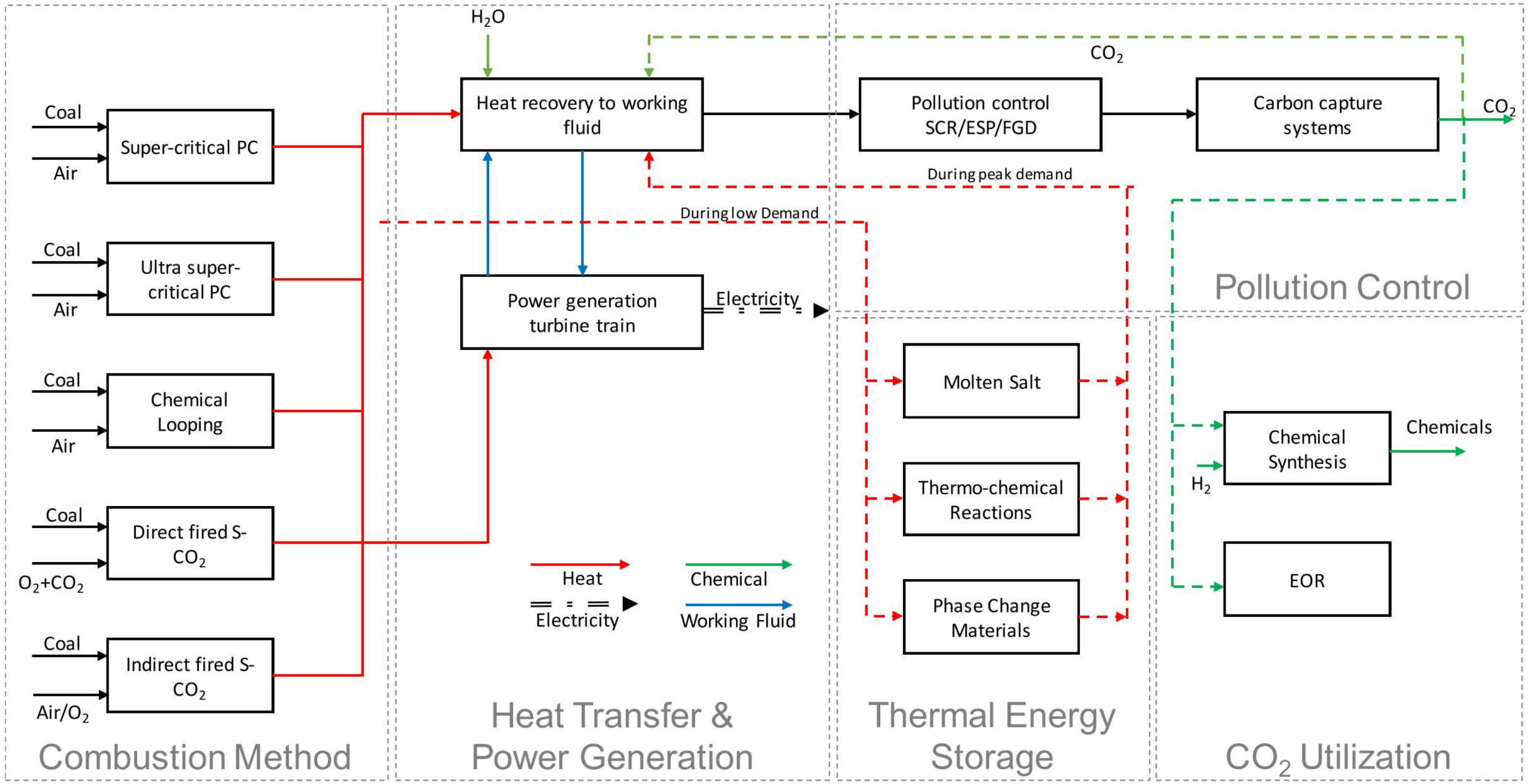
Part 2: Conceptual Design and the Coal FIRST Initiative

- **F**lexible operation
  - High ramp rates and minimum load operation
- **I**nnovative design
  - > 40% HHV efficiency, near zero emissions
- **R**esilient operation
  - Minimize forced outages
- **S**mall scale
  - <400 MW, minimize field construction costs
- **T**ransformative technologies
  - Coupled with energy storage



IDAES Vision: Provide next-generation computational tools and apply them to the design of these transformative energy solutions

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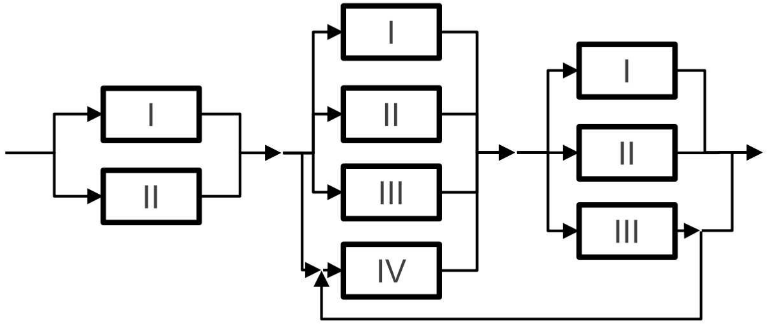
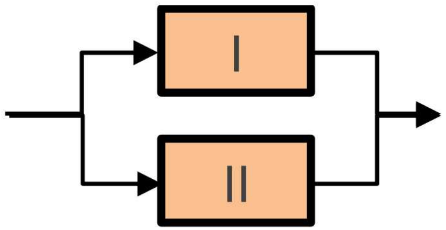
PyoSyn Framework in IDAES

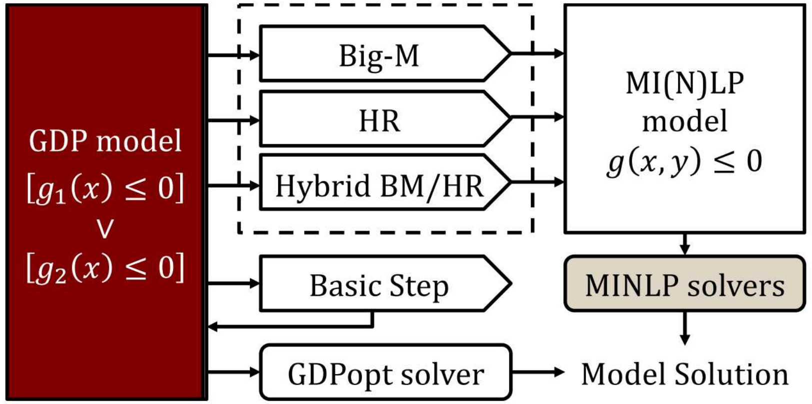


IDAES Modeling Framework



$$\begin{bmatrix} Y_1 \\ g_1(x) \le 0 \end{bmatrix} \vee \begin{bmatrix} Y_2 \\ g_2(x) \le 0 \end{bmatrix}$$

Pyomo.GDP Disjunctive Modeling



General GDP Solution Approaches

- Models built using IDAES framework and process model library
- High-level representation of superstructure with disjunctions
- Automatic conversion to MINLP with Pyomo.GDP
- Pyomo.GDP framework allows reformulation to MINLP
  - Automatic conversion to MINLP – fewer modeling errors
  - Gives access to general MINLP solvers

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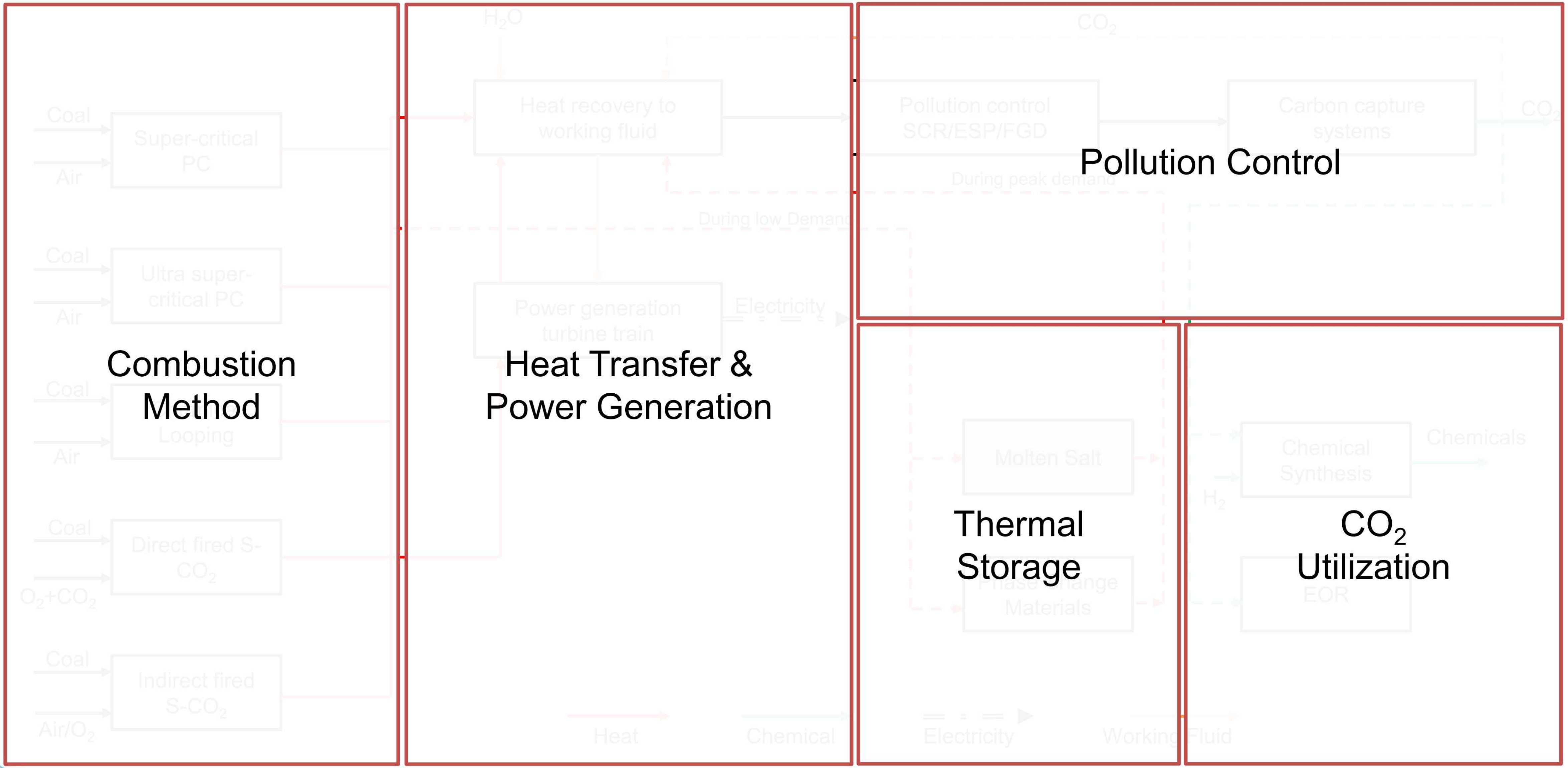
PYOMO GDP

Example Superstructure for Next Generation Coal Plants



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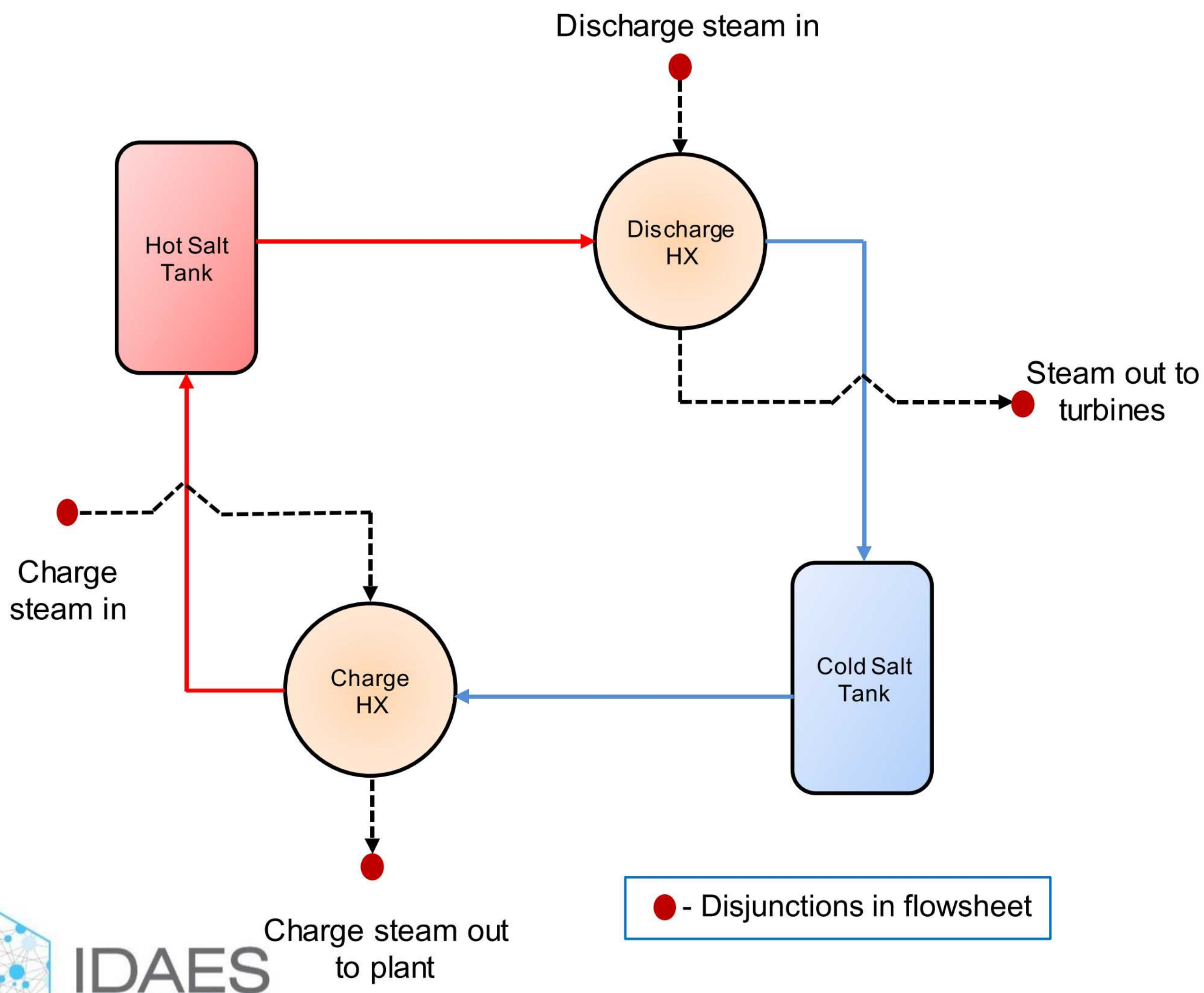
Case study: Thermal Energy Storage Design Problem

Molten Salt Storage Flowsheet



Case study objectives

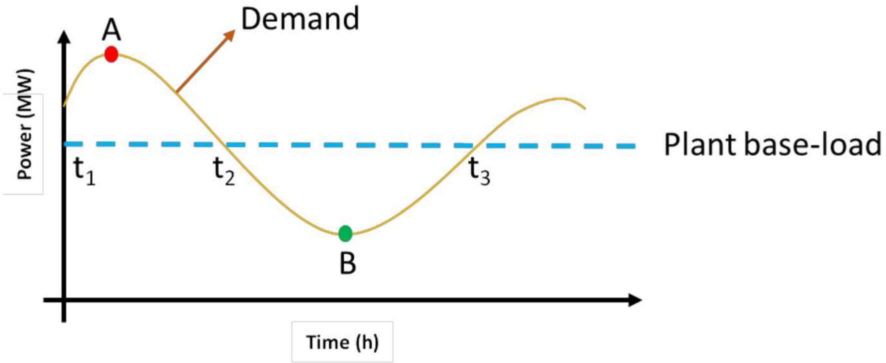
- Design a plant retrofit to enhance flexibility for a notional base-load plant by adding a thermal storage system
- Use standard IDAES models
- Solve using GDPopt
- Identify API challenges

Demand and base-load information

- Base-load: 615 MW
- PA demand data scaled to 615 MW

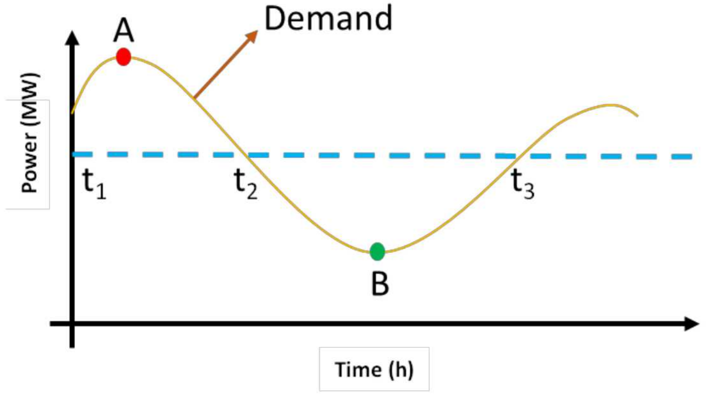
Optimization variables

- Design: Heat Exchanger Area, Tank Volume
- Operating: Flow rate of steam, salt
- Discrete decisions: Type of Salt, Steam extraction points, Steam return points

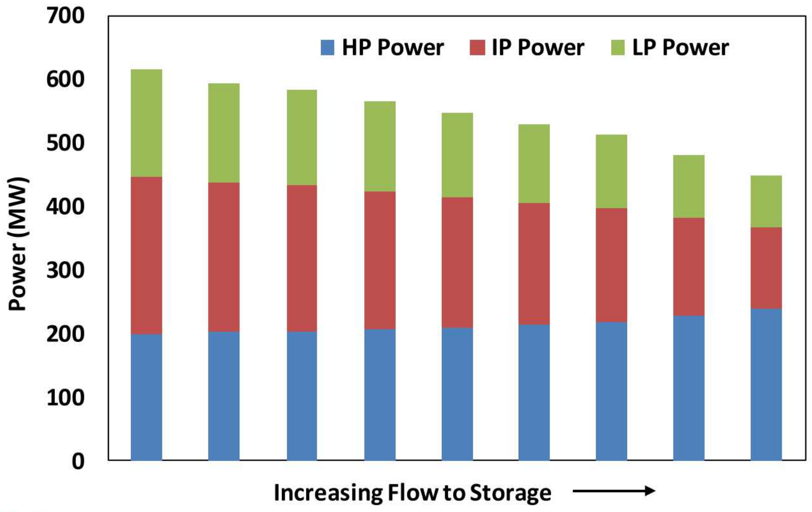


Case study: Thermal Energy Storage

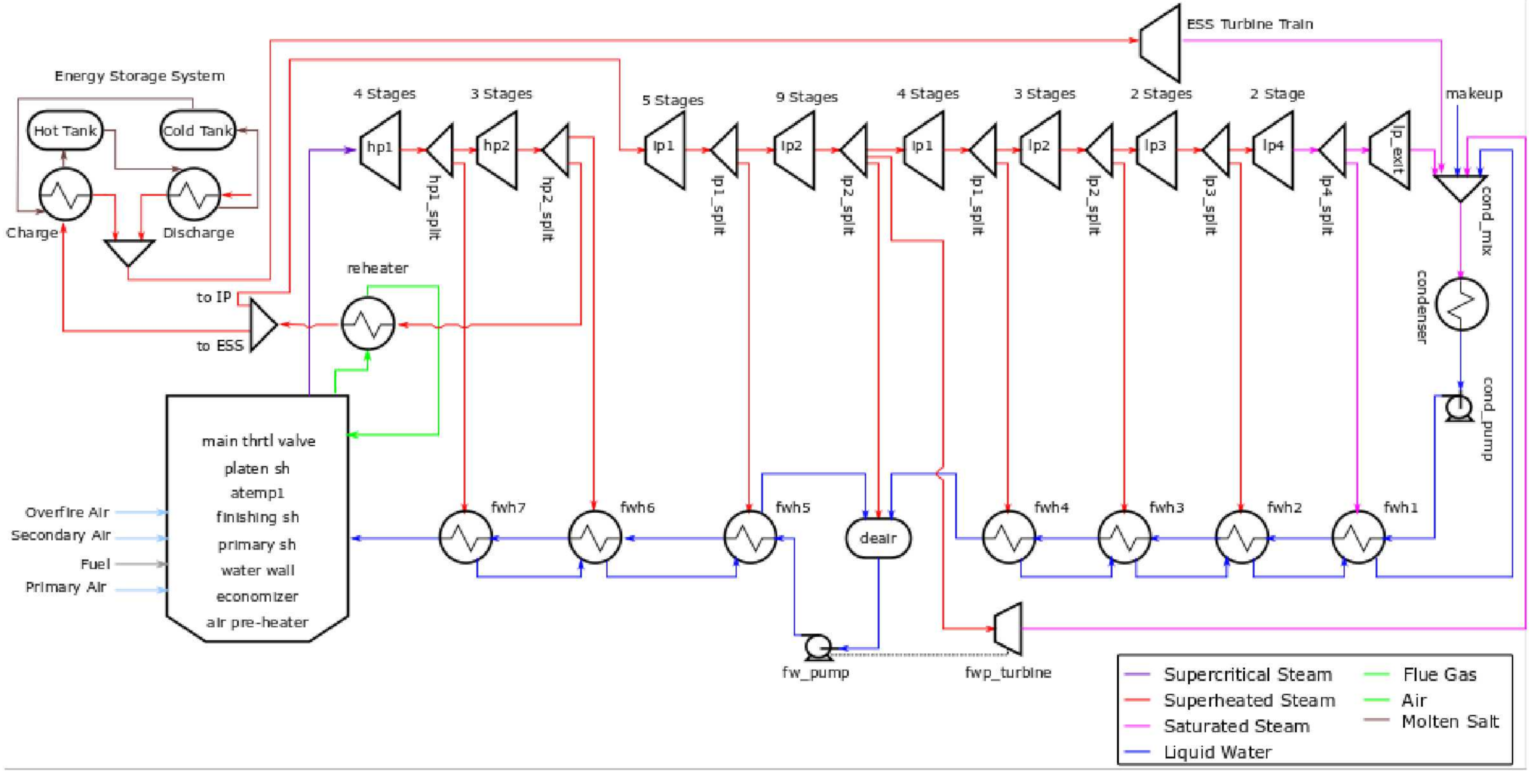
Integrated Storage for Flexibility



Base-load power output



Base-load + thermal energy storage system simulation



- Design of storage system integrated with existing coal plant
- Discrete decisions: Steam extraction / return points, storage medium
- Formulation: IDAES models with disjunctions on units
- Solved with logic-based, outer-approximation in GDPOpt

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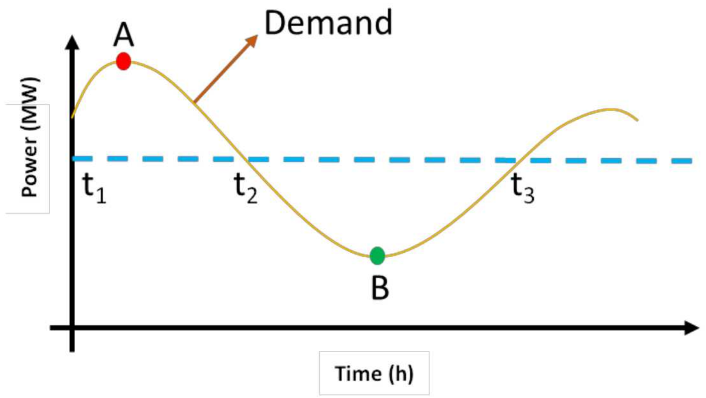
Case study: Thermal Energy Storage

Integrated Storage for Flexibility



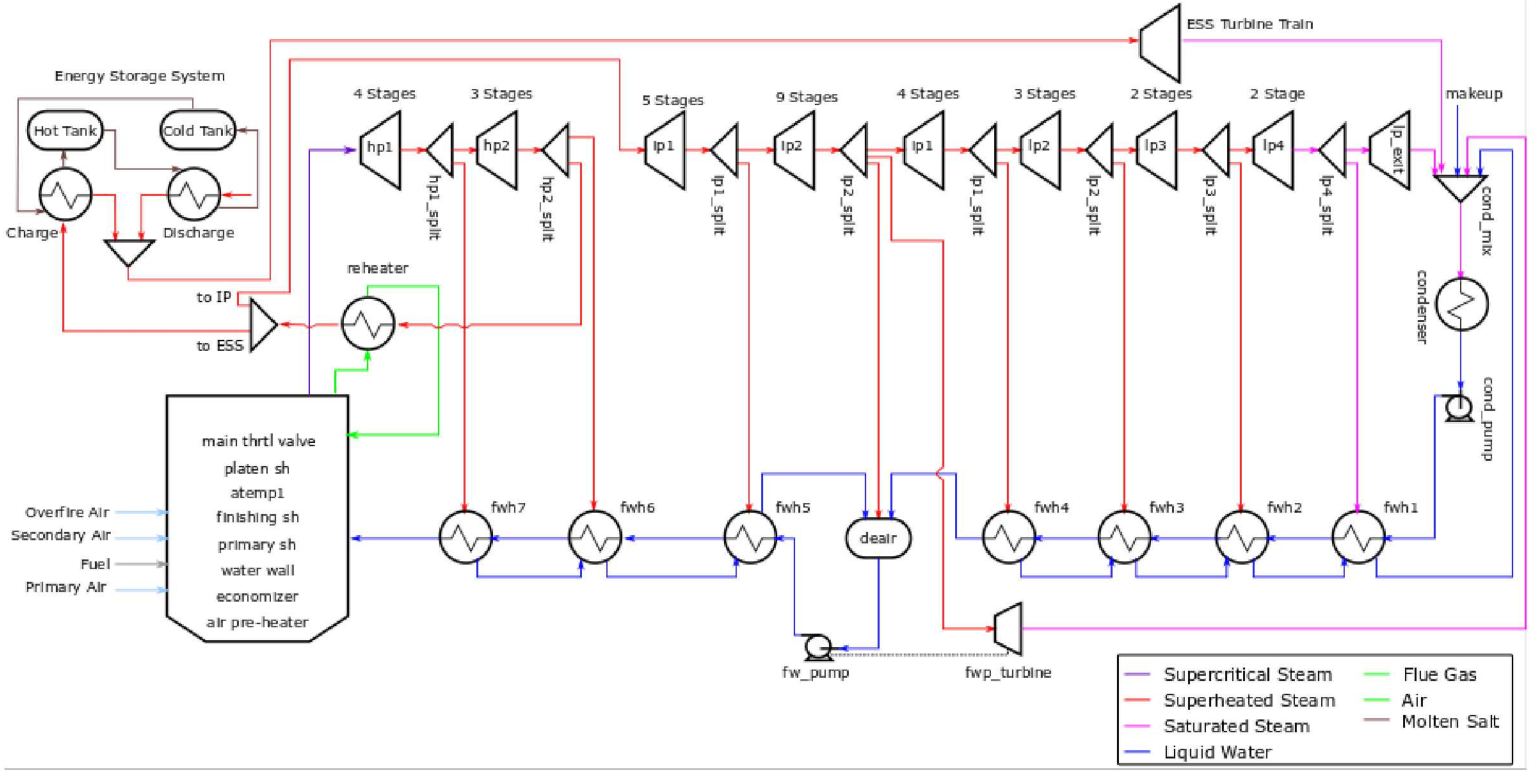
Design: Zero ramp rate, base-load plant

Max. surplus (deficit) power = 99 (79) MW

Design Variable	Opt. Value
Salt Inventory (MT)	4,530
Volume of tanks (m^3)	2,390
Charge HX area (m^2)	1,360
Discharge HX area (m^2)	1,270

Operating Variable	Optimal Value
Steam flow: max. charge (discharge)	5.89 (8.83) kg-mol/s
Salt flow: max. charge (discharge)	195 (155) kg/s

Base-load + thermal energy storage system simulation

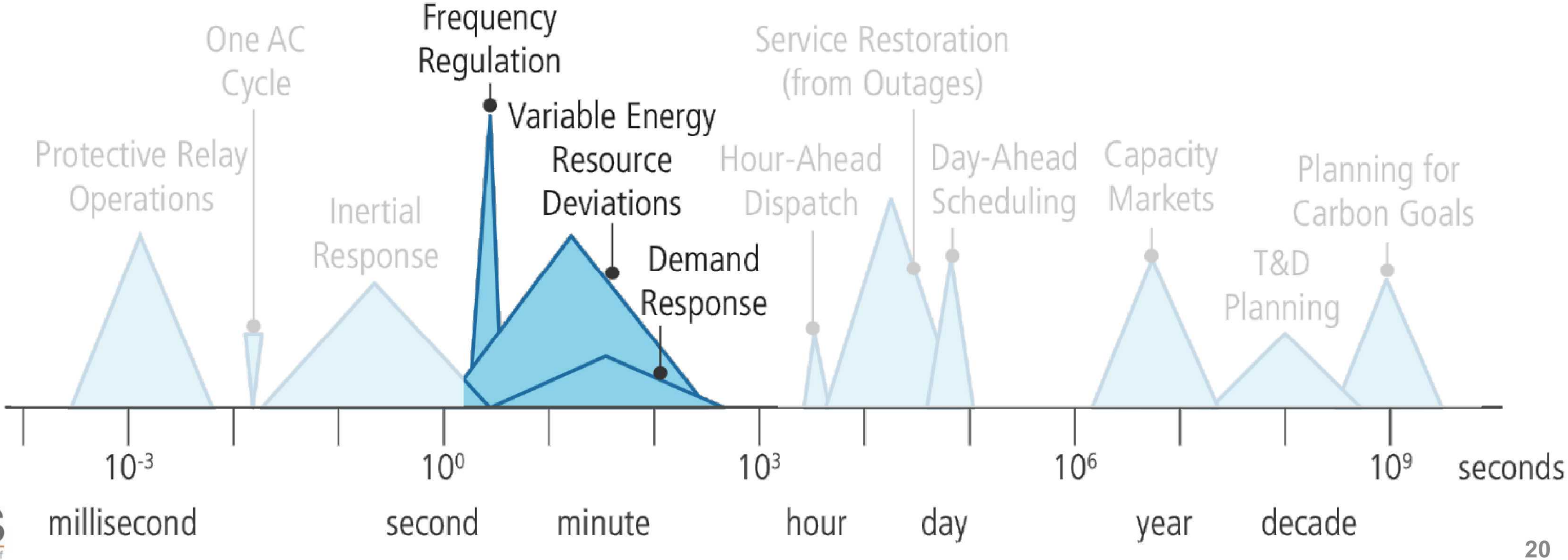


- Design of storage system integrated with existing coal plant
- Discrete decisions: Steam extraction / return points, storage medium
- Formulation: IDAES models with disjunctions on units
- Solved with logic-based, outer-approximation in GDPOpt

Part 3: Power systems / market interactions

Improving individual generator economics requires **co-optimizing control and market participation decisions**.

- How to manage market uncertainty and price volatility?
- How to systematically balance revenue and equipment health?
- How to design/debottleneck energy systems to better exploit markets?



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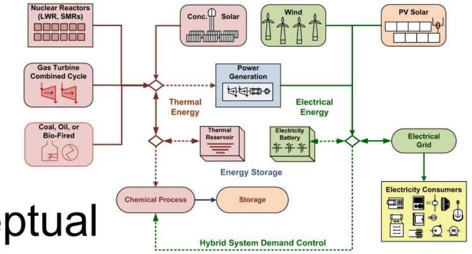
Integrated market participation models

High-Fidelity Analysis

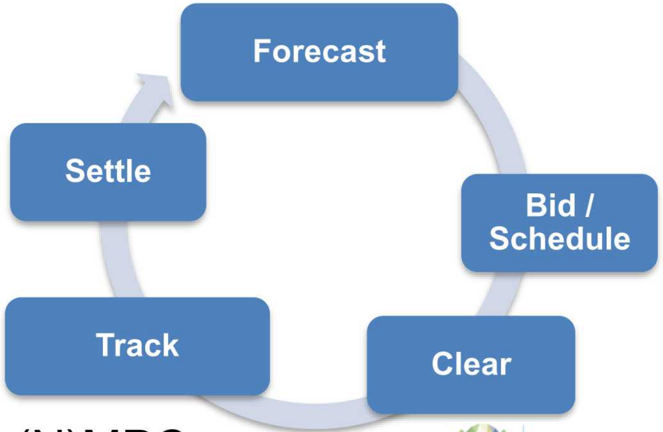
Dynamic Modeling & Optimization



Conceptual Design

Data Reconciliation

Market Participation



(N)MPC

PRESCIENT

Grid Modeling

Expansion Planning

Grid / Market Simulation

Understanding how generators interact with the power system

- Elucidate complex relationships between resource dynamics and market dispatch (with uncertainty, beyond price-taker assumption)
- Guide conceptual design / retrofit to meet current and future power grid needs

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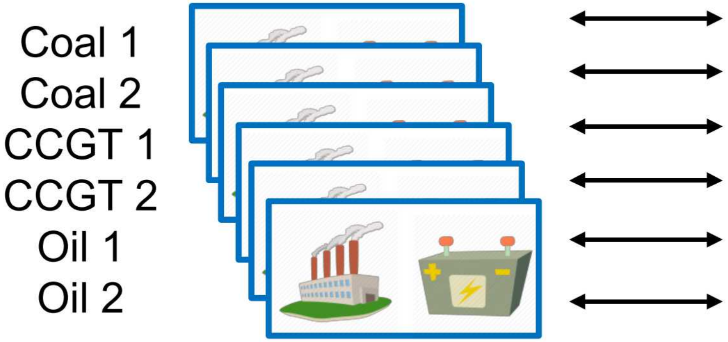
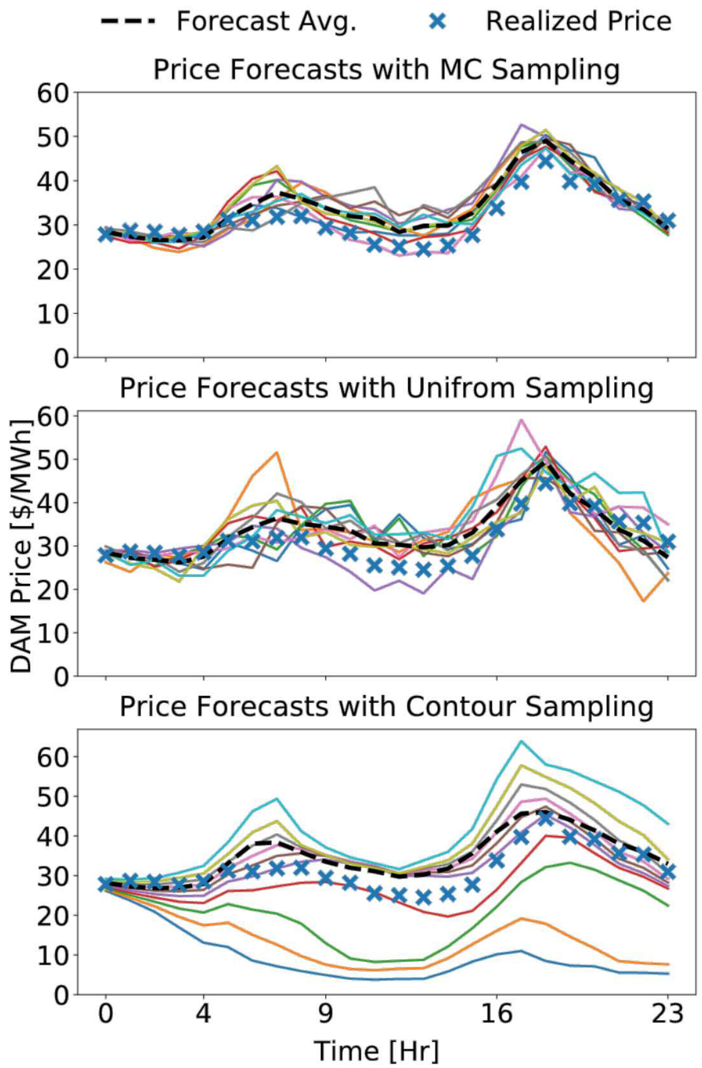
Case study: thermal generators with energy storage

- Evaluate the impact of pairing thermal generators with electricity storage



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

Forecast: Sampling strategies



Increasing emphasis on tail scenarios

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Quantifying the opportunity of integrated analysis

Model	Participation Mode	Perfect Information	MC Sampling	Uniform Sampling	Contour Sampling
Thermal Generators	**Bid Curve**	$ 51,804,073.72 (100%)	$ 46,238,387.27 (89.26%)	$ 47,313,418.39 (91.33%)	$ 47,502,696.98 (91.70%)
	Self-schedule		$ 42,089,244.93 (81.25%)	$ 41,048,765.19 (79.24%)	$ 41,257,593.30 (79.64%)
Thermal Generators + Storage	**Bid Curve**	$ 54,125,108.97 (100%)	$ 46,646,203.30 (86.18%)	$ 48,178,307.90 (89.01%)	$ 47,936,761.15 (88.57%)
	Self-schedule		$ 43,586,149.56 (80.53%)	$ 41,319,371.66 (76.34%)	$ 42,476,495.25 (78.48%)

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

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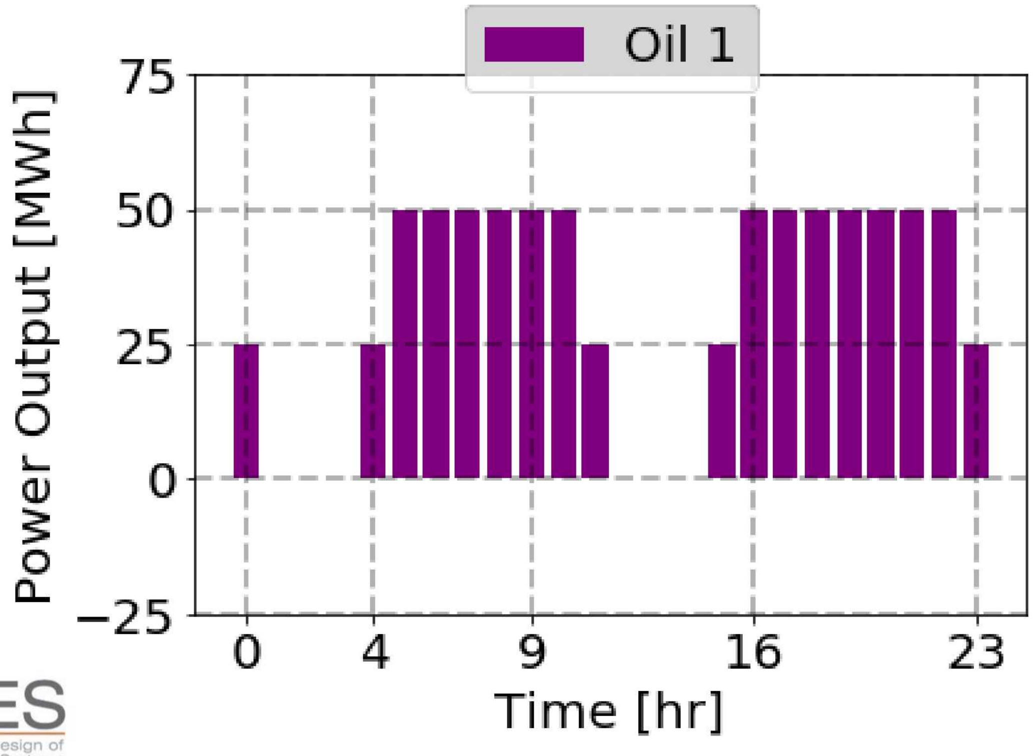
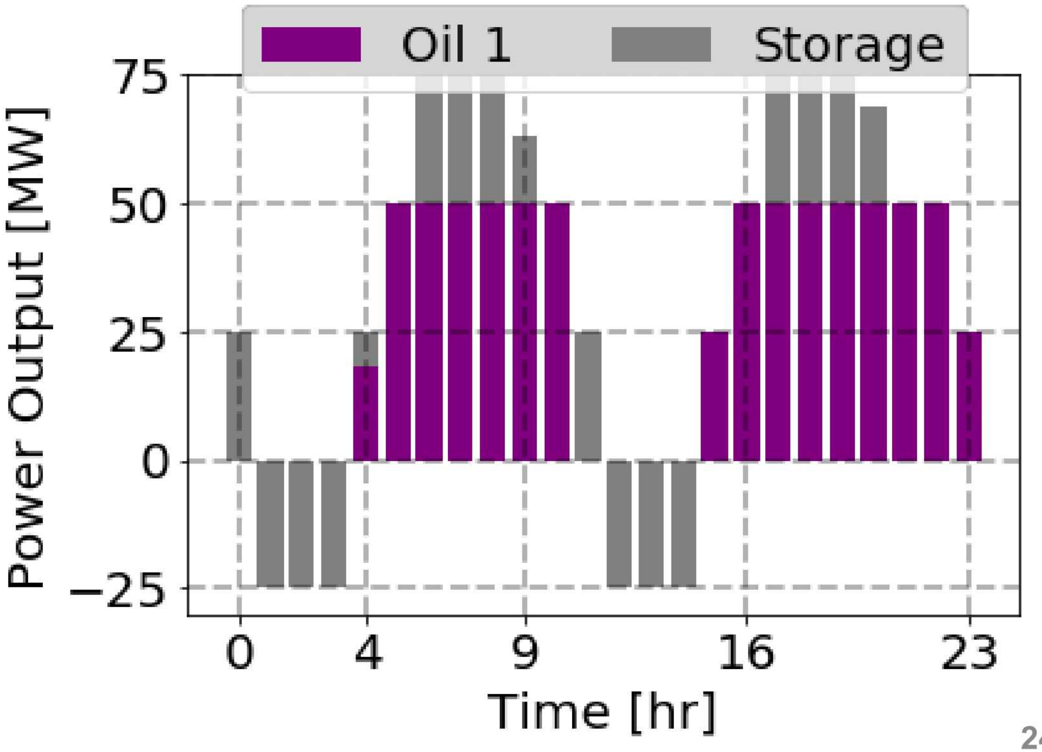
Quantifying the impact on a single generator

- Consider a single generator, "Oil 1"
  - Smaller (50 MW) marginal generator, 25 MW (100 MWh) storage
    - Generator alone: $1.87M net revenue
    - Generator + storage: $2.57M net revenue
  - (assuming perfect information)





Summary

- IDAES has been developing sophisticated modeling, analysis, and optimization tools to support the design, modeling, and optimization of advanced energy systems.
- IDAES enables a complete workflow from rigorous analysis to system-wide optimization.
- The IDAES team is applying these tools in several areas, including
  - Supporting existing fossil generation systems
  - Designing new hybrid generation systems
  - Evaluating new technologies in the context of the broader power system

- How to get involved
  - Stakeholder Advisory Board
  - Download the software
  - Collaborate with the IDAES team
    - e.g. through Cooperative Research and Development Agreements (CRADA)
  - Join the IDAES development community

Next SAB meeting: May 5-7 2020, Crystal City, VA

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The IDAES Technical Team:

- **National Energy Technology Laboratory**: David Miller, Tony Burgard, John Eslick, Andrew Lee, Miguel Zamarripa, Jinliang Ma, Dale Keairns, Jaffer Ghouse, Emmanuel Ogbe, Gary Kocis, Ben Omell, Chinedu Okoli, Richard Newby, Grigorios Panagakos, Maojian Wang, Andres Calderon, Naresh Susarla
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- **Lawrence Berkeley National Laboratory**: Deb Agarwal, Dan Gunter, Keith Beattie, John Shinn, Hamdy Elgammal, Joshua Boverhof, Karen Whitenack, Oluwamayowa (Mayo) Amusat, Makayla Shepherd
- **Carnegie Mellon University**: Larry Biegler, Nick Sahinidis, Chrysanthos Gounaris, Ignacio Grossmann, Owais Sarwar, Natalie Isenberg, Chris Hanselman, Marissa Engle, Qi Chen, Cristiana Lara, Robert Parker, Ben Sauk, Vibhav Dabadghao, Can Li, David Molina Thierry
- **West Virginia University**: Debangsu Bhattacharyya, Paul Akula, Anca Ostace, Quang-Minh Le
- **University of Notre Dame**: Alexander Dowling, Xian Gao

The Tri-State/Escalante Technical and Engineering Team:

- **Tri-State G&T**: Indrajit Bhattacharya, Sean Mann; **Escalante**: Brian Rychener, Tim Hoisington, Phillip Pinkston

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